Supporting Information

I_2-Triggered N-O Cleavage of Ketoxime Acetates for the Synthesis of 3-(4-Pyridyl)indoles

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[b]*School of International education, Xinxiang Medical University, Xinxiang, Henan 453003, P. R. China.*
[c]*School of Pharmacy, Key Laboratory of Molecular Pharmacology and Drug Evaluation, Ministry of Education, Collaborative Innovation Center of Advanced Drug Delivery System and Biotech Drugs in Universities of Shandong, Yantai University, Shandong, Yantai 264005, P. R. China.*

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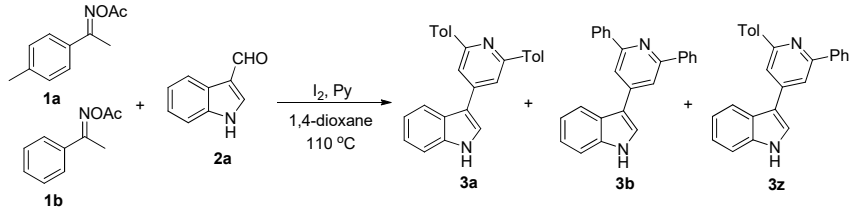
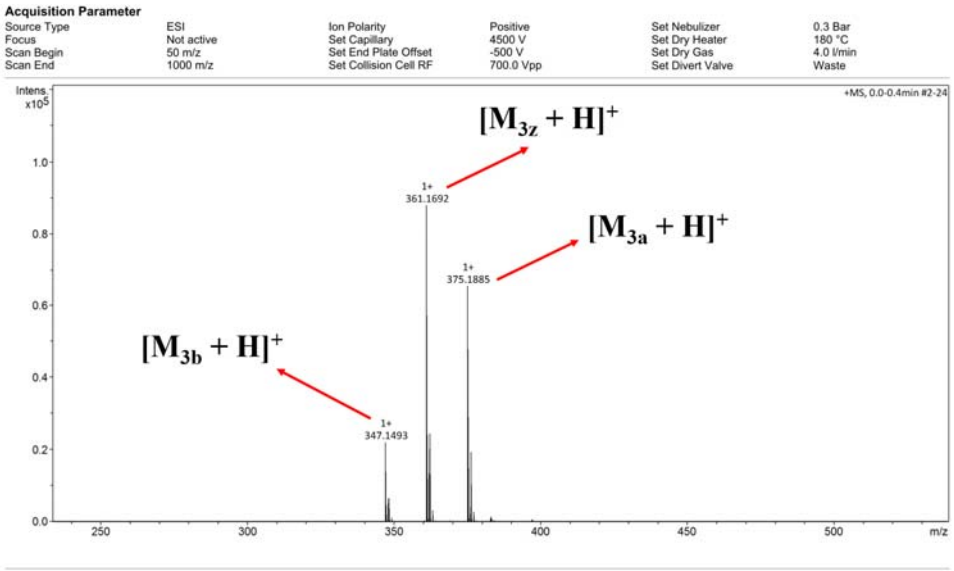
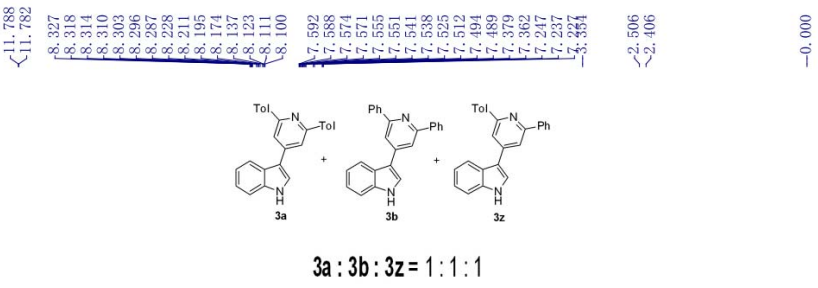
1. The cross-coupling reaction

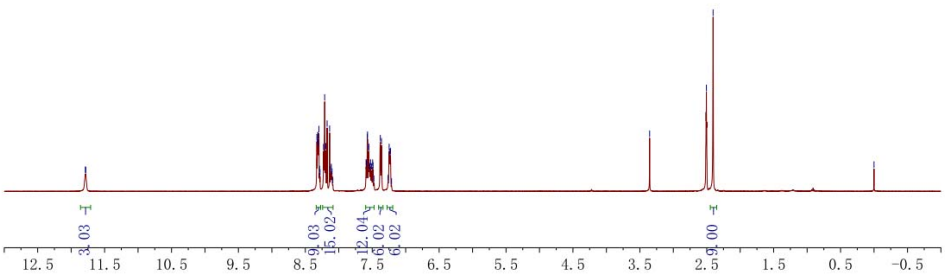
In order to further confirm our proposed mechanism, we investigated the cross-coupling reaction between two representative substrates 4-methylacetophenone oxime acetate (**1a**) and acetophenone oxime acetate (**1b**) under standard conditions. Fortunately, all the products were successfully identified by HRMS analysis of the crude reaction extract, and the ratio of **3a**, **3b** and **3z** further calculated by ^{1}H NMR analysis.







3a : 3b : 3z = 1 : 1 : 1



2. Crystallographic data and molecular structure of compounds 3o

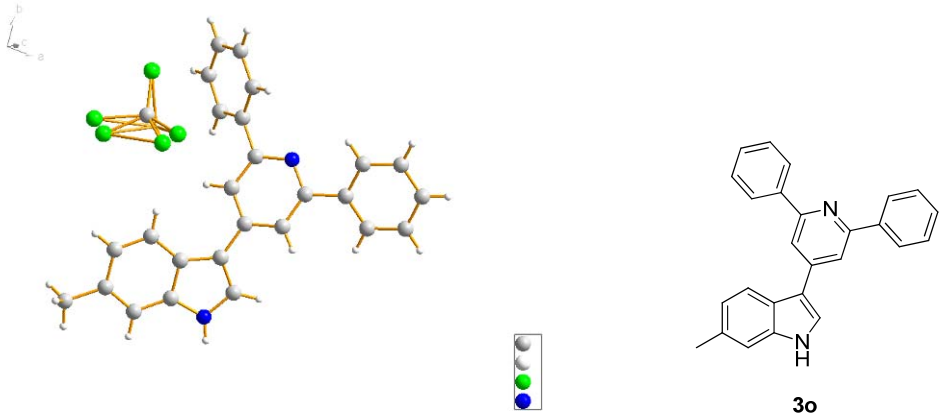
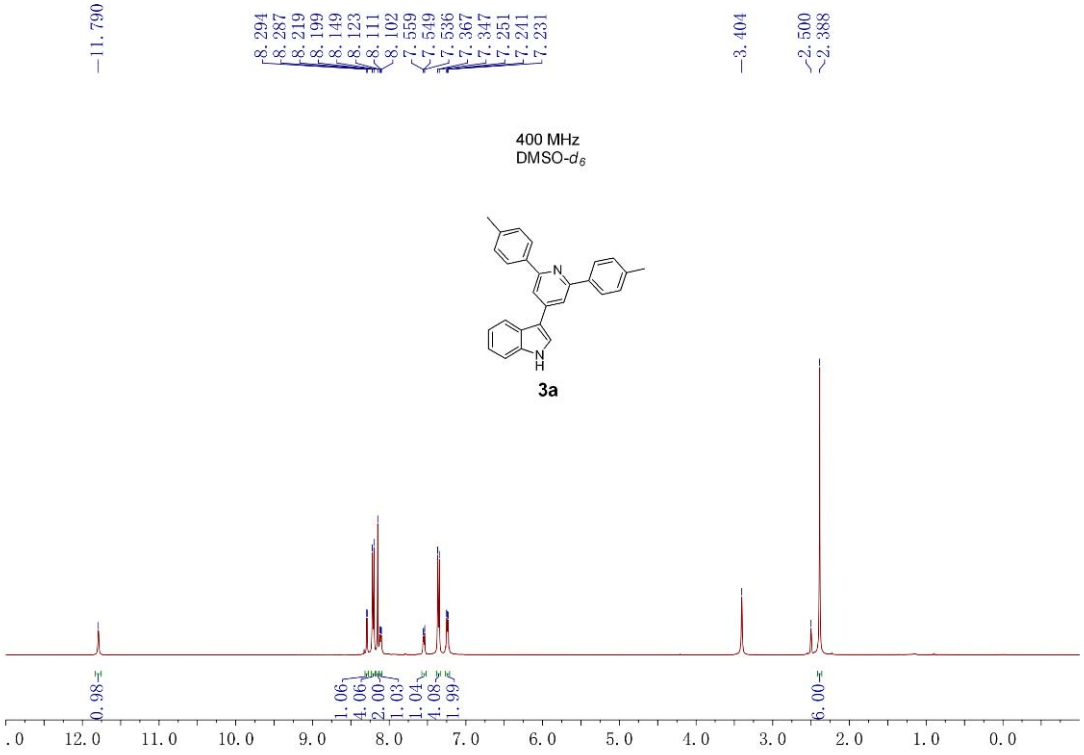
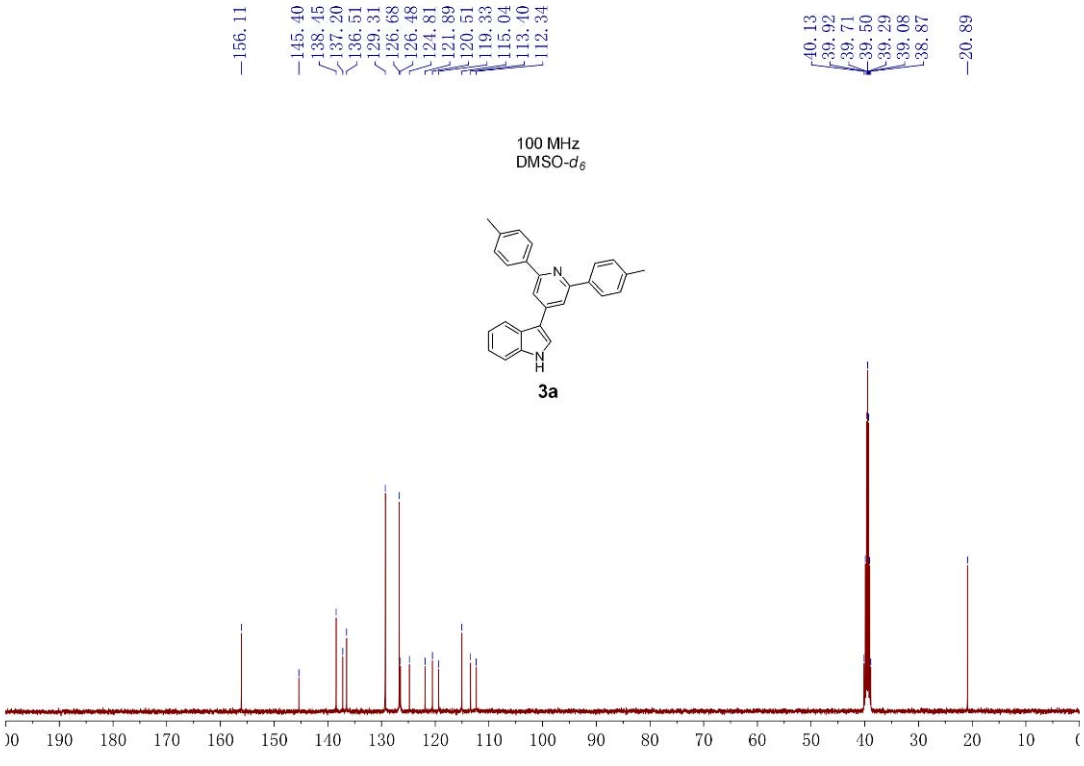


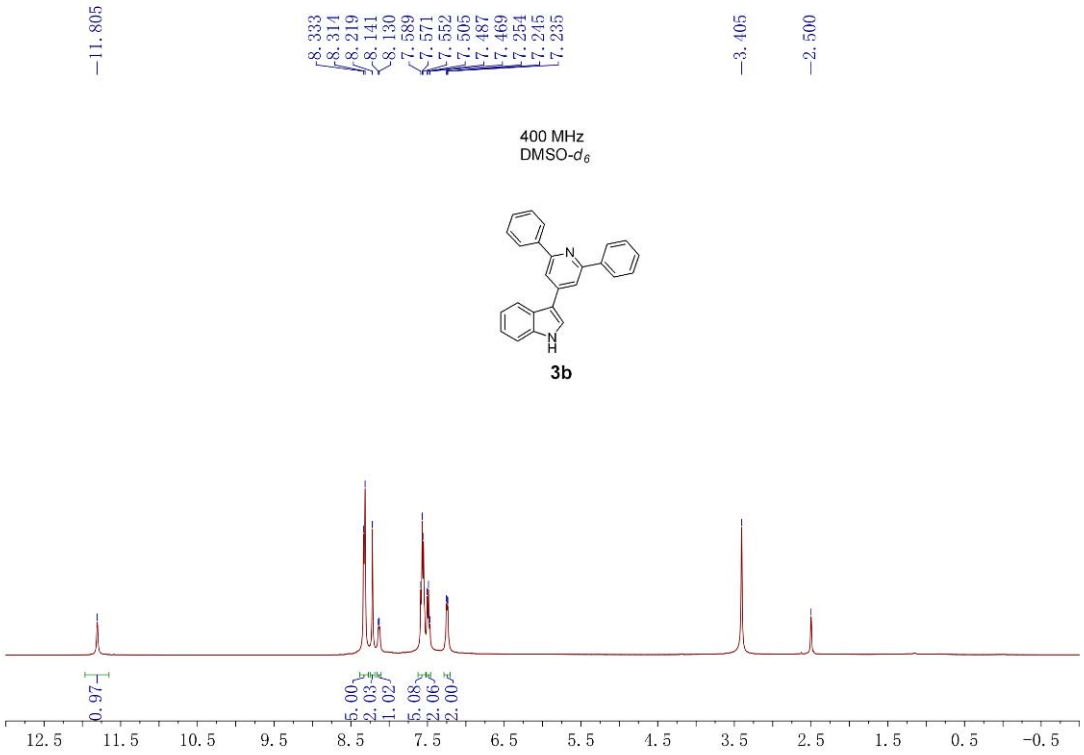
Figure S1. X-ray crystal structure of **3o** (CCDC: 1844843)

Empirical formula	$C_{53}H_{41}Cl_3N_4$ [2(C_{26} H_{20} N_2), $CHCl_3$]		Absorption coefficient	2.210 mm^{-1}
Formula weight	840.25		F(000)	1752
Temperature	293(2) K		Crystal size	0.220 x 0.200 x 0.180 mm^3
Wavelength	1.54178 Å		Theta range for data collection	3.536 to 74.902°
Crystal system	Monoclinic		Reflections collected	8719
Space group	C2/c		Independent reflections	4174 [R(int) = 0.0231]
Unit cell dimensions	a = 25.4646(15) Å	α = 90°	Refinement method Full	Full-matrix least-squares on F^2
	b = 16.7733(9) Å	β= 100.998(6)°	Data / restraints / parameters	4174 / 30 / 290
	c = 10.4497(8) Å	γ = 90°	Goodness-of-fit on F2	1.071
Volume	4381.4(5) $Å^3$		Final R indices [I>2sigma(I)]	R1 = 0.0801, wR2 = 0.2265
Z	4		R indices (all data)	R1 = 0.0900, wR2 = 0.2487
Density (calculated)	1.274 Mg/m^3		Largest diff. peak and hole	0.504 and -0.682 $e.Å^{-3}$

3. ^{1}H and ^{13}C NMR spectra of compounds 3 and 5



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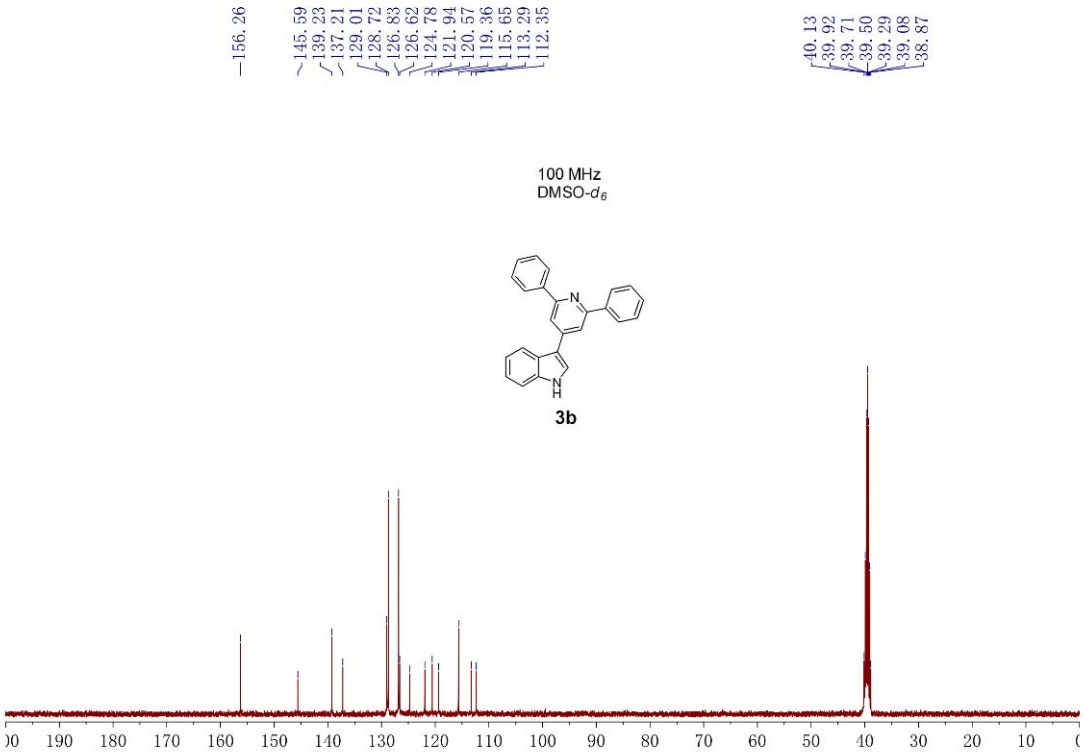
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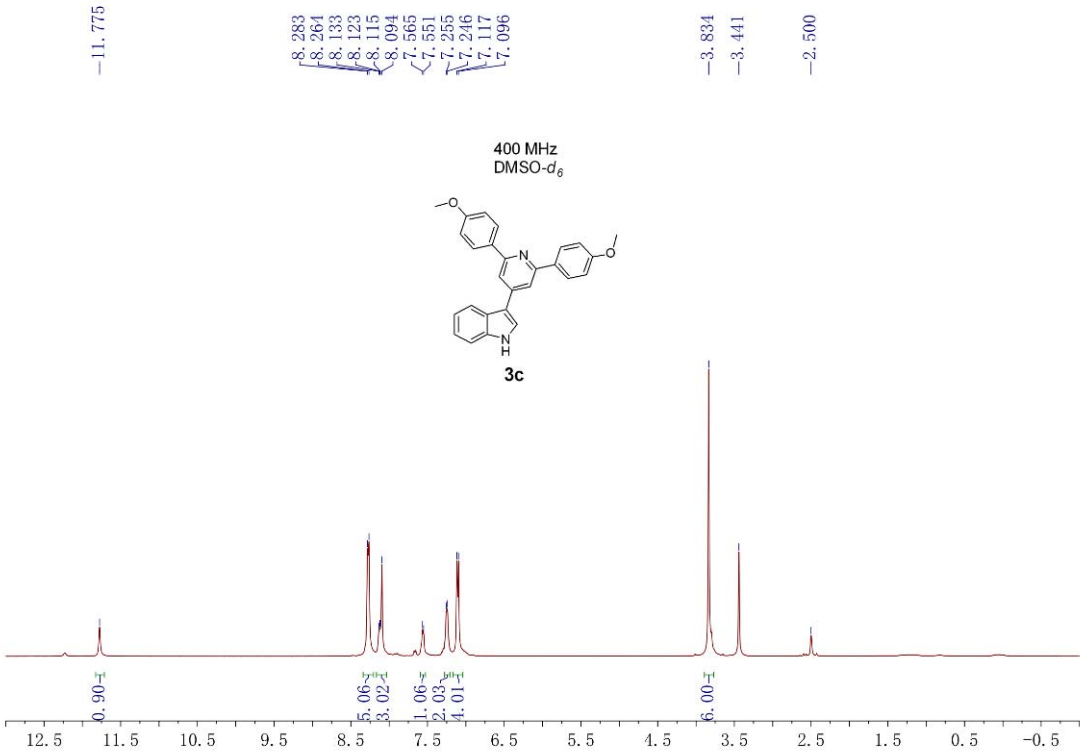
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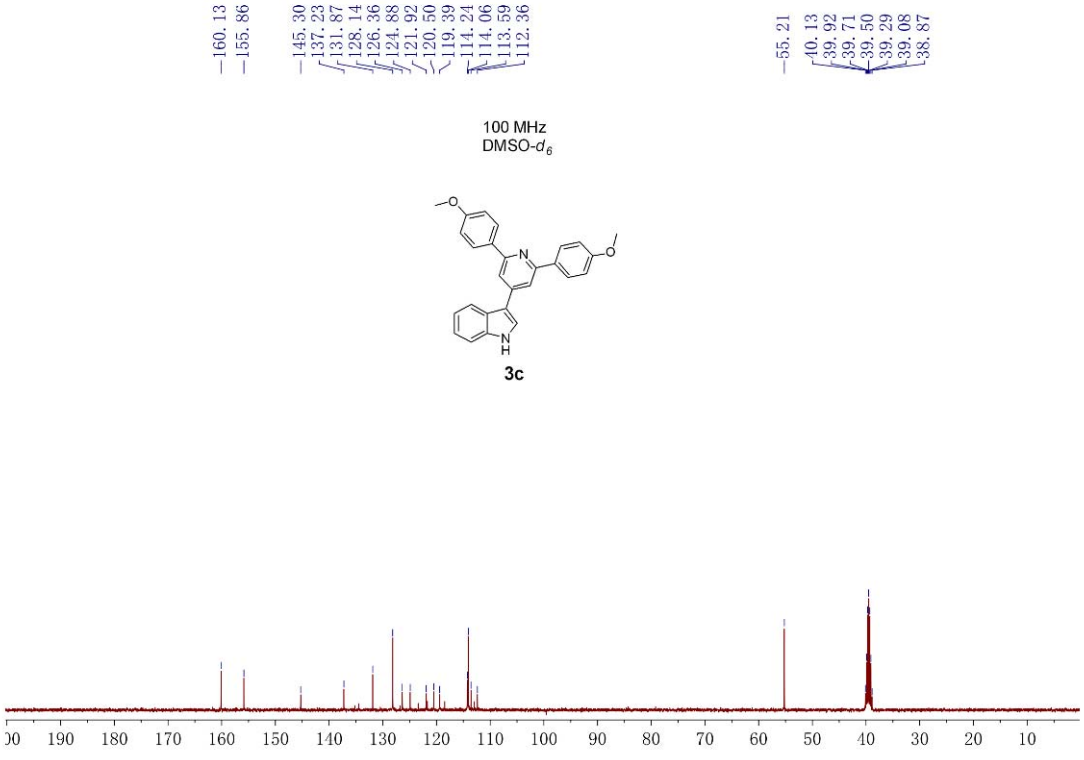
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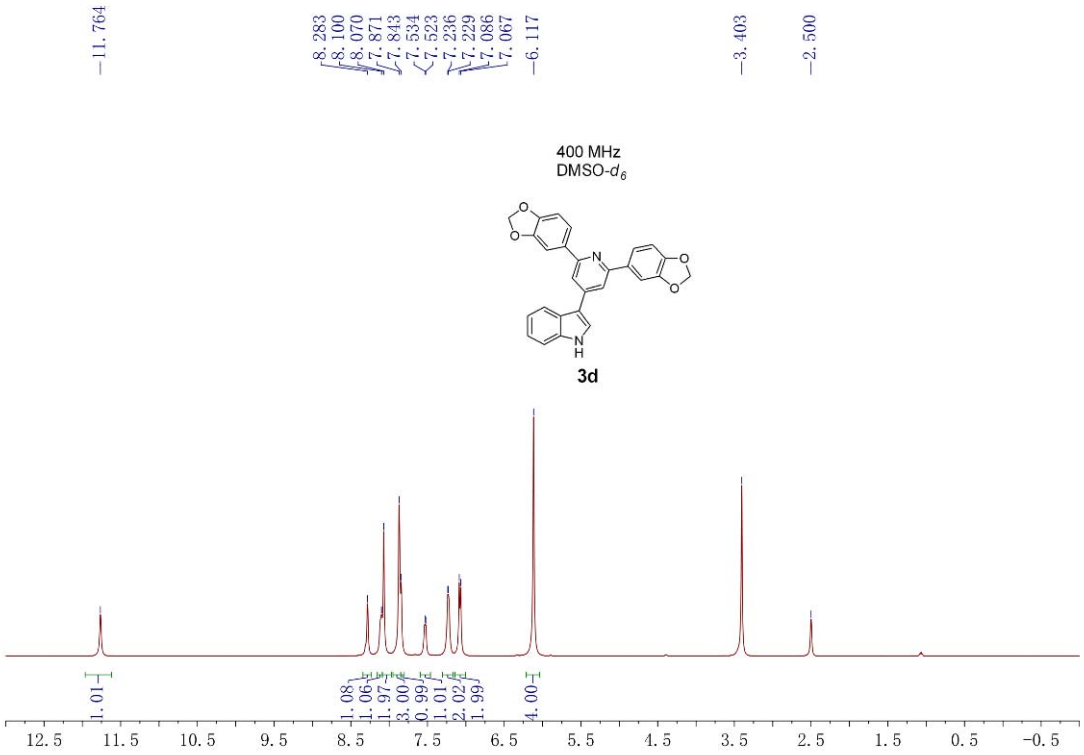
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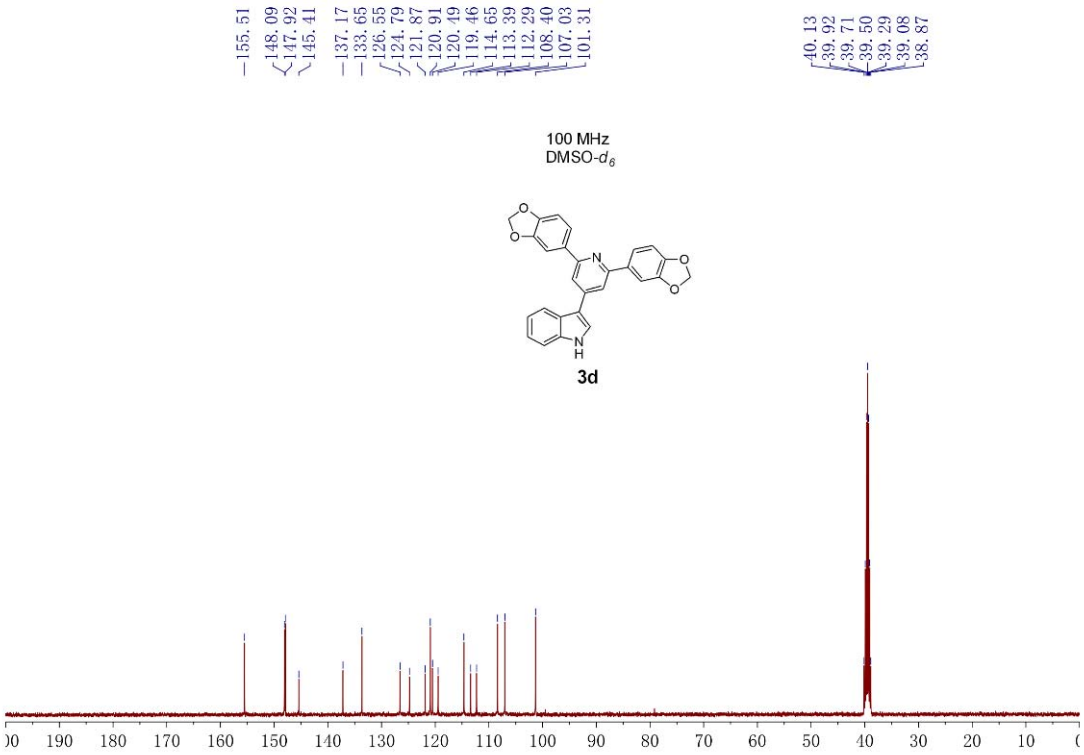
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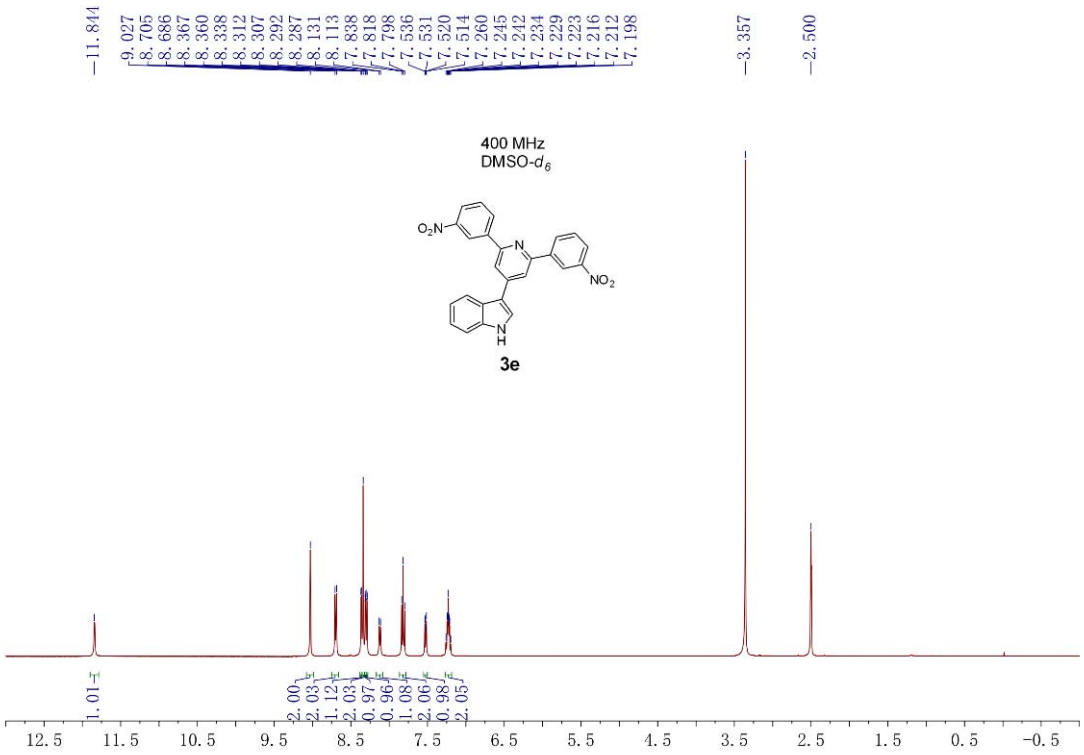
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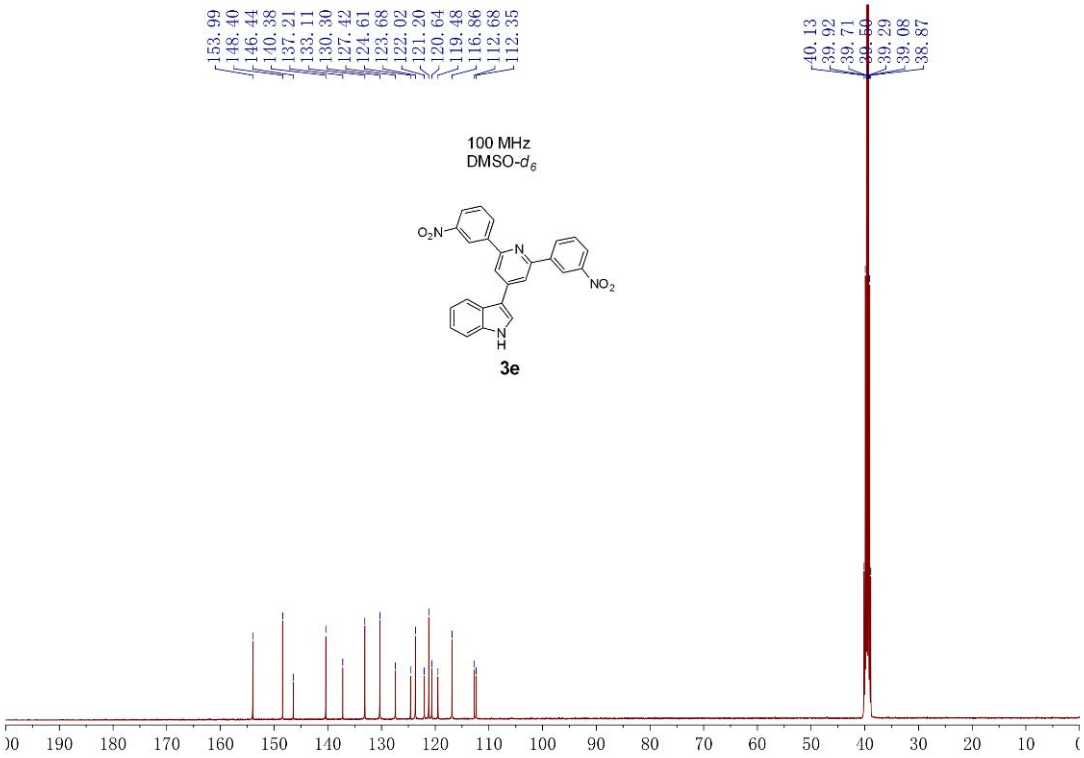
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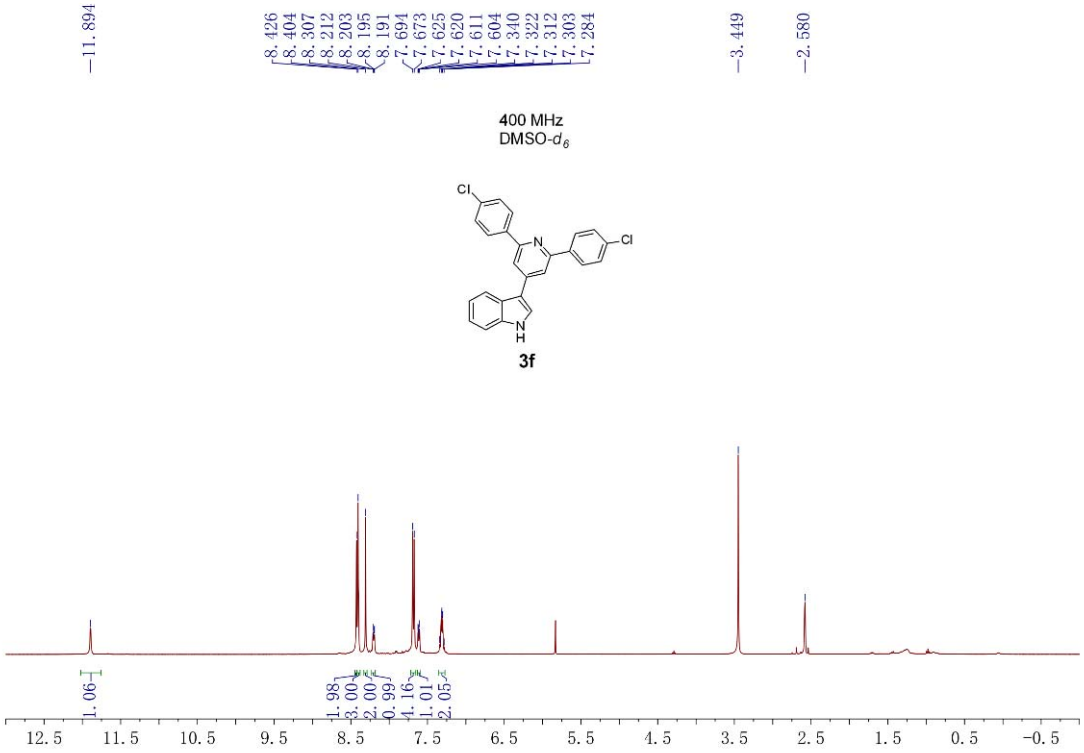
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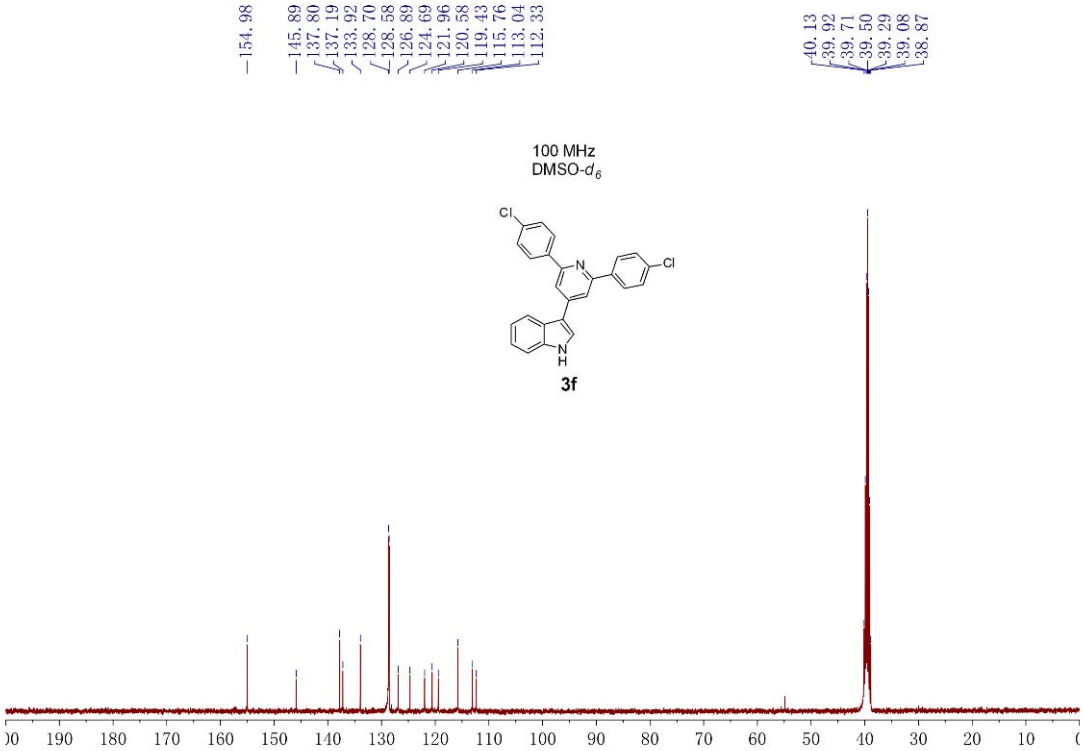
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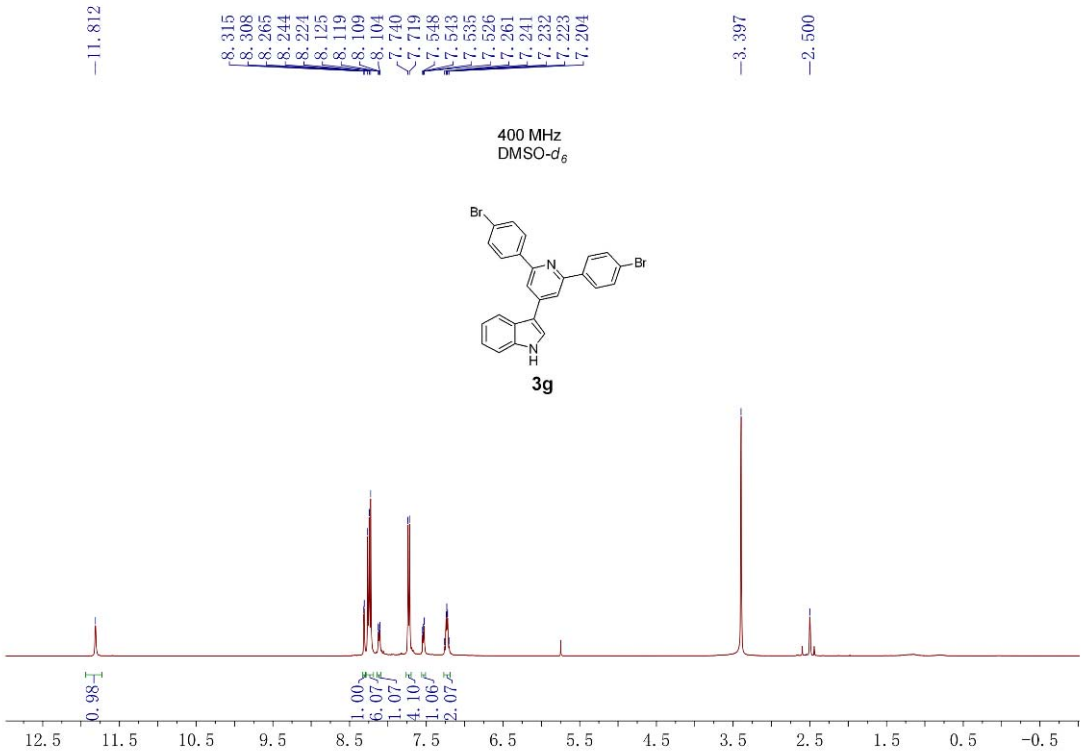
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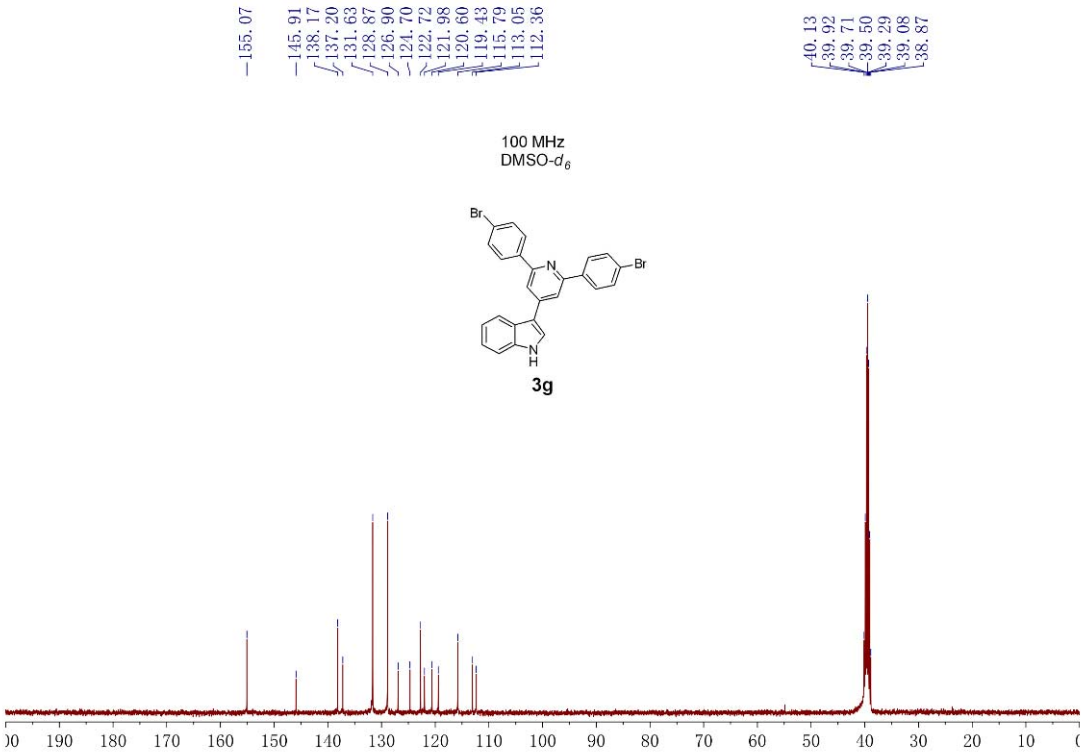
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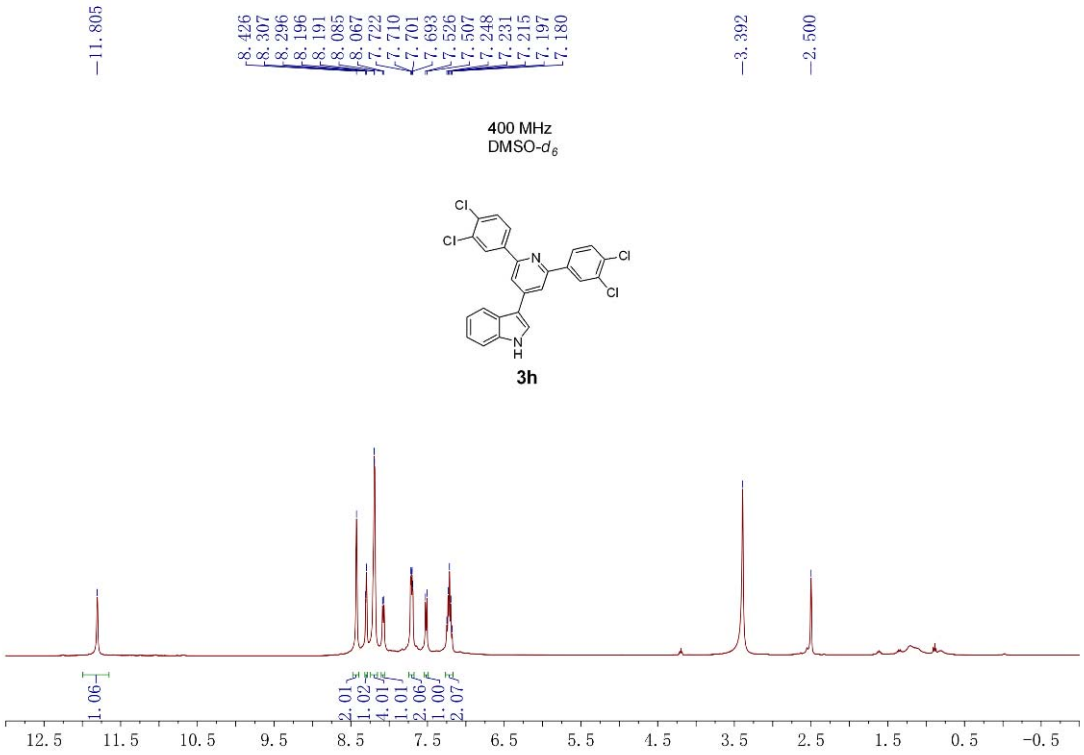
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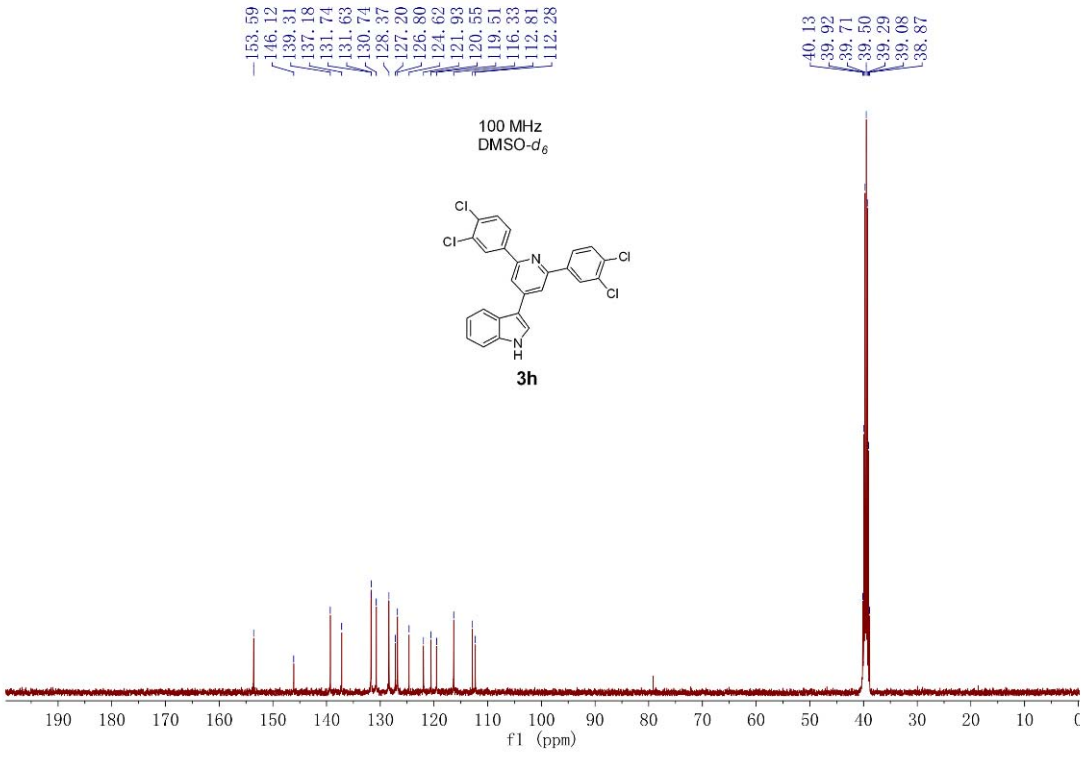
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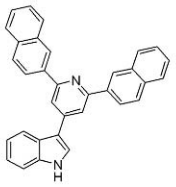

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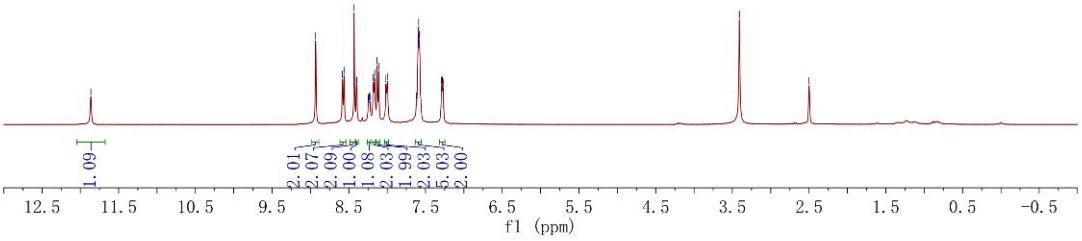

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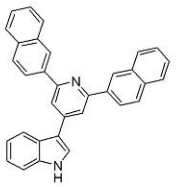

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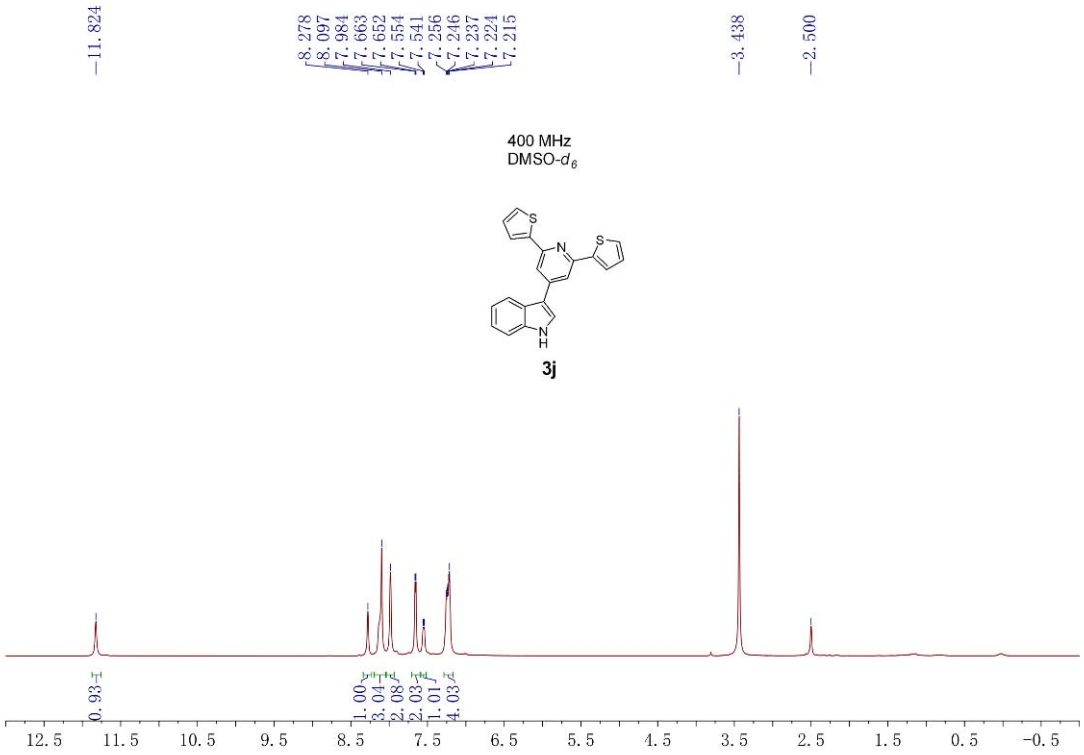
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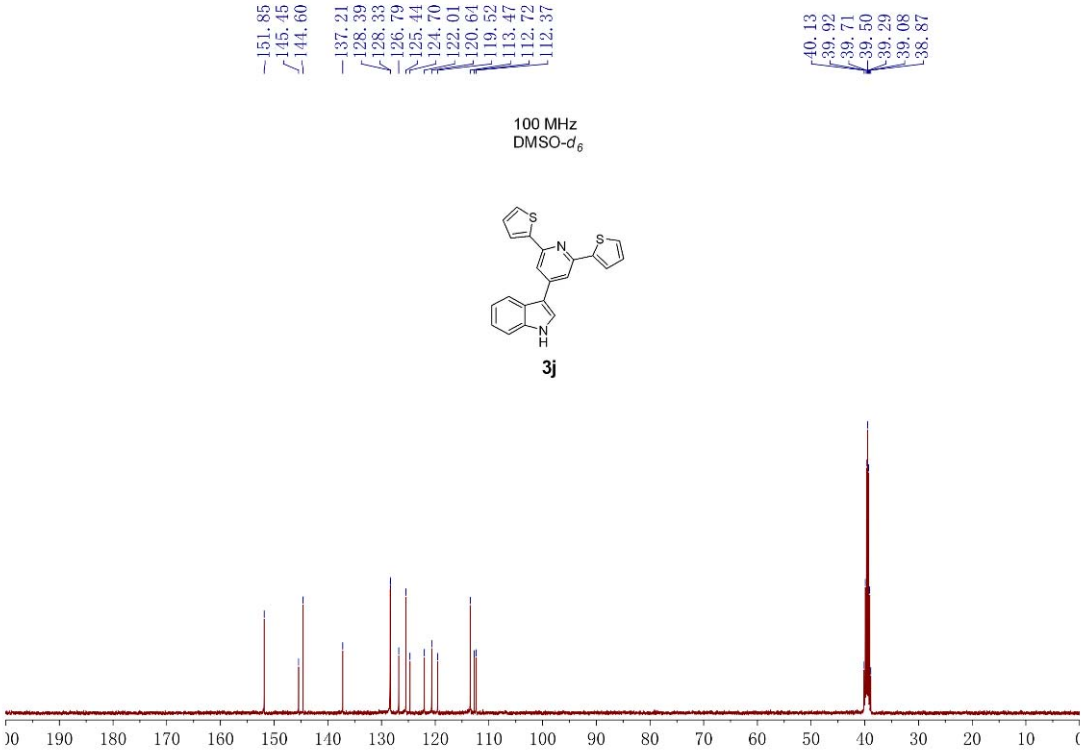
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100 MHz
DMSO-d_6
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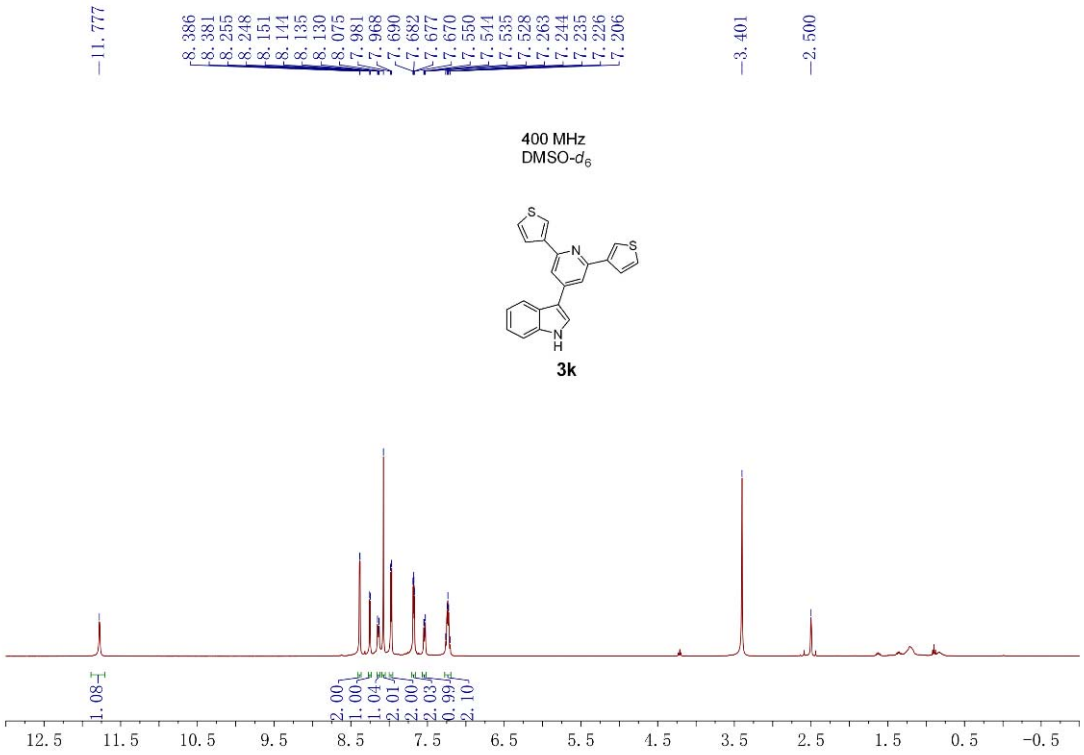
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2.5
1.5
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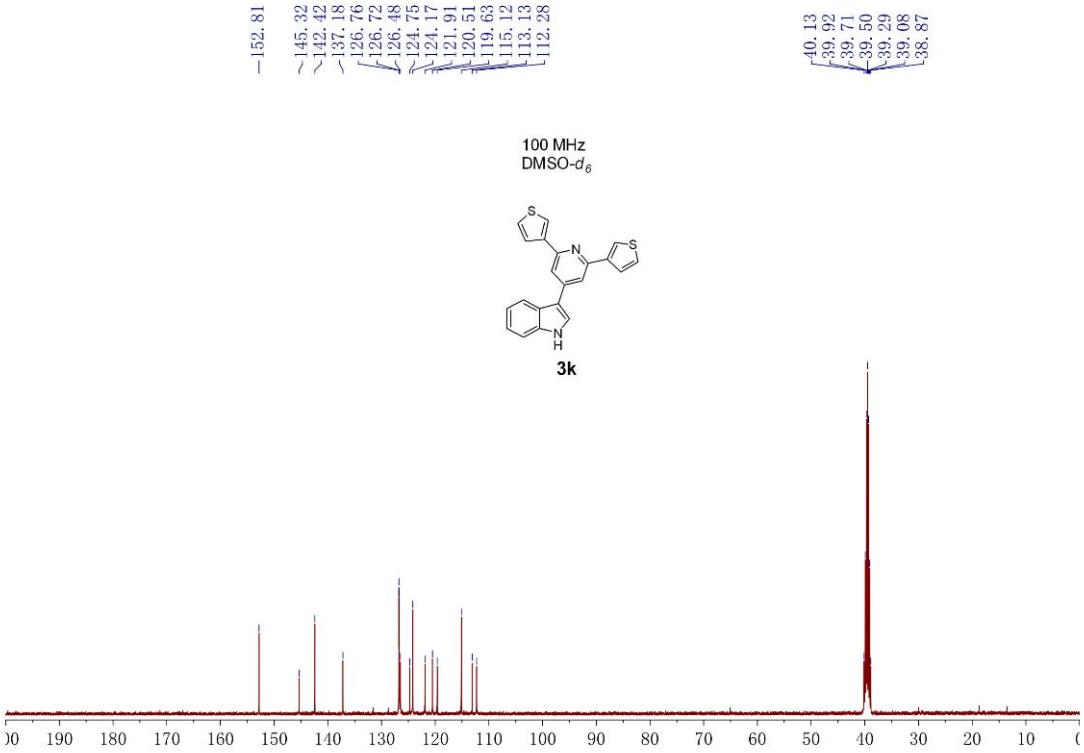
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126.48
124.75
124.17
121.91
120.51
119.63
115.12
113.13
112.28
40.13
39.92
39.71
39.50
39.29
39.08
38.87
100 MHz
DMSO-d_6
3k
190
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150
140
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120
110
100
90
80
70
60
50
40
30
20
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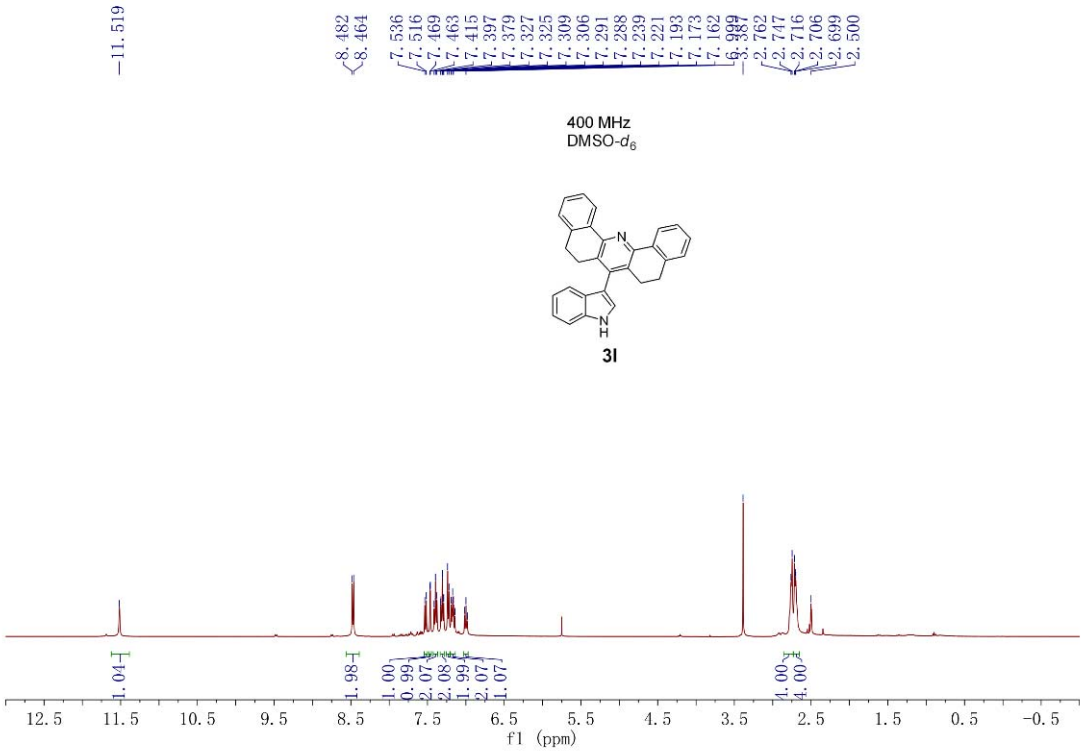
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8.482
8.464
7.536
7.516
7.469
7.463
7.415
7.397
7.379
7.327
7.325
7.309
7.306
7.291
7.288
7.239
7.221
7.193
7.173
7.162
3.387
2.762
2.747
2.716
2.706
2.699
2.500
400 MHz
DMSO-d_6
3l
1.04
1.98
1.00
0.99
2.07
2.08
1.99
2.07
1.07
4.00
4.00
12.5
11.5
10.5
9.5
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6.5
5.5
4.5
3.5
2.5
1.5
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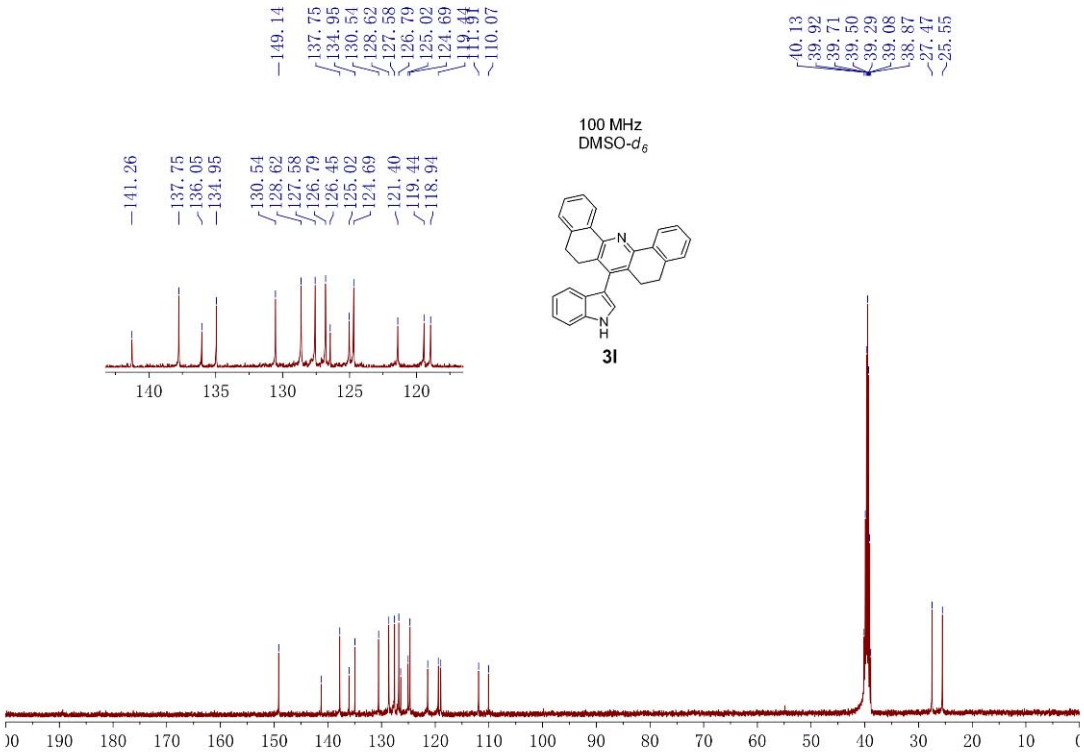
f1 (ppm)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127.58
126.79
125.02
124.69
119.44
118.94
110.07
40.13
39.92
39.71
39.50
39.29
39.08
38.87
27.47
25.55
100 MHz
DMSO-d_6
141.26
137.75
136.05
134.95
130.54
128.62
127.58
126.79
126.45
125.02
124.69
121.40
119.44
118.94
3l
140
135
130
125
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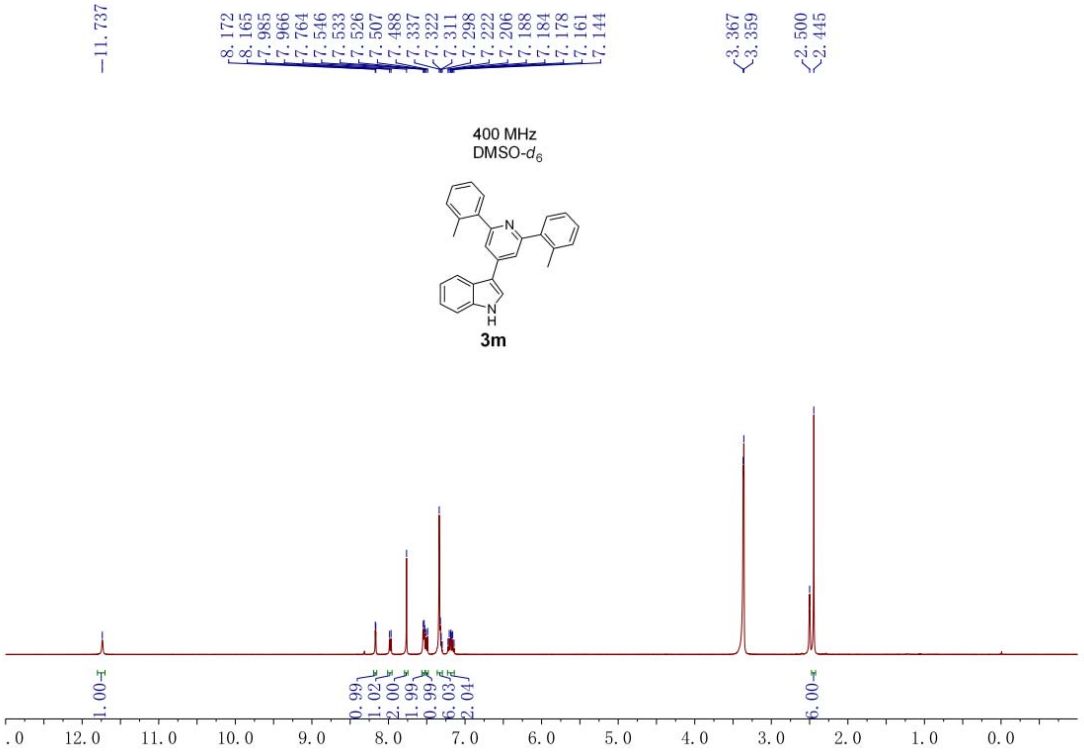
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8.165
7.985
7.966
7.764
7.546
7.533
7.526
7.507
7.488
7.337
7.322
7.311
7.298
7.222
7.206
7.188
7.184
7.178
7.161
7.144
3.367
3.359
2.500
2.445
400 MHz
DMSO-d_6
3m
1.00
0.99
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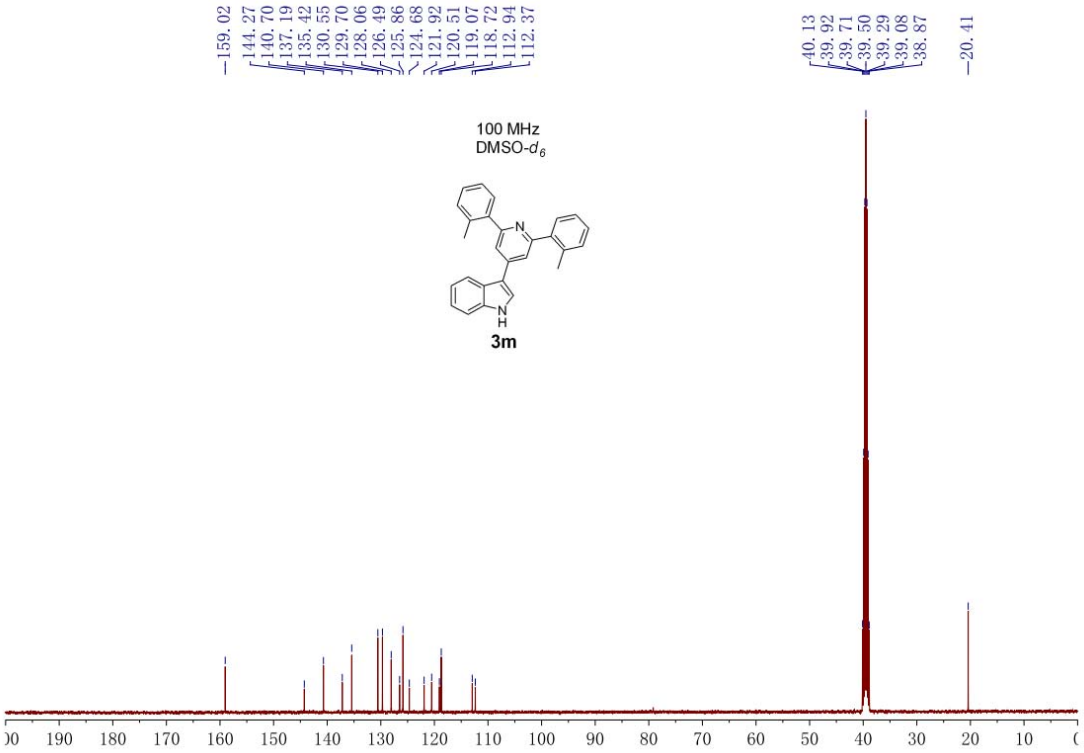
2.00
1.99
0.99
6.03
2.04
6.00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144.27
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137.19
135.42
130.55
129.70
128.06
126.49
125.86
124.68
121.92
120.51
119.07
118.72
112.94
112.37
40.13
39.92
39.71
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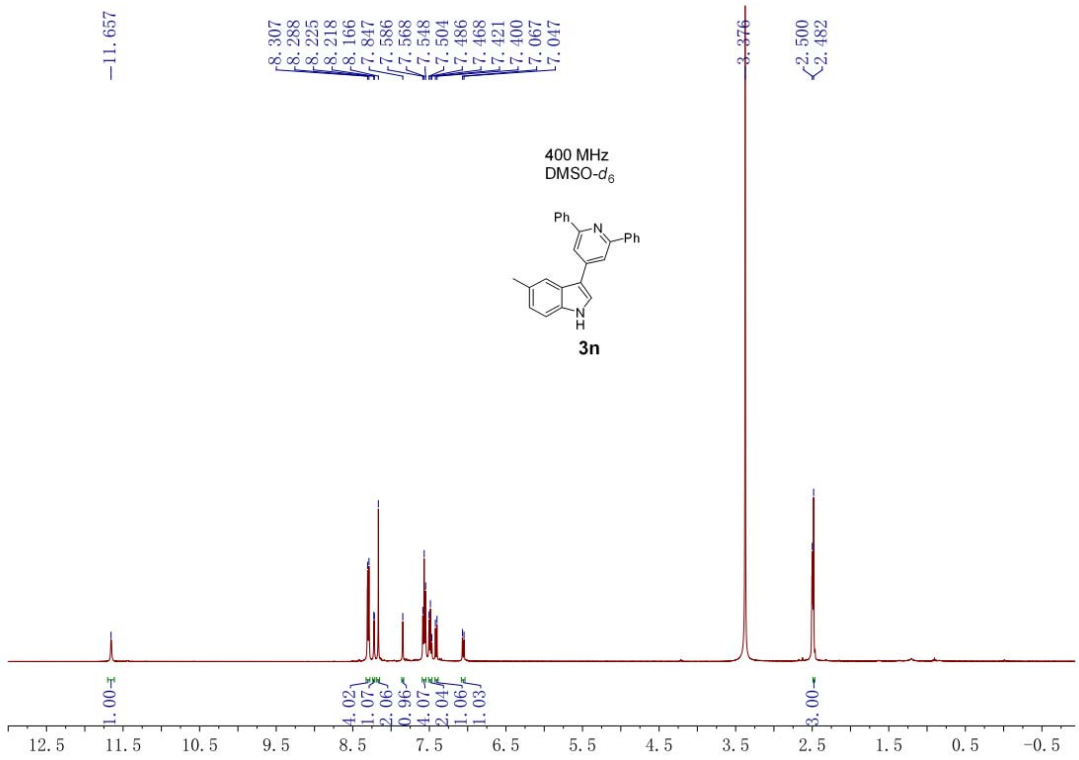
39.29
39.08
38.87
20.41
100 MHz
DMSO-d_6
3m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8.288
8.225
8.218
8.166
7.847
7.586
7.568
7.548
7.504
7.486
7.468
7.421
7.400
7.067
7.047
3.376
2.500
2.482
400 MHz
DMSO-d_6
Ph
N
Ph
N
H
3n
1.00
4.02
1.07
2.06
0.96
4.07
2.04
1.06
1.03
3.00
12.5
11.5
10.5
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8.5
7.5
6.5
5.5
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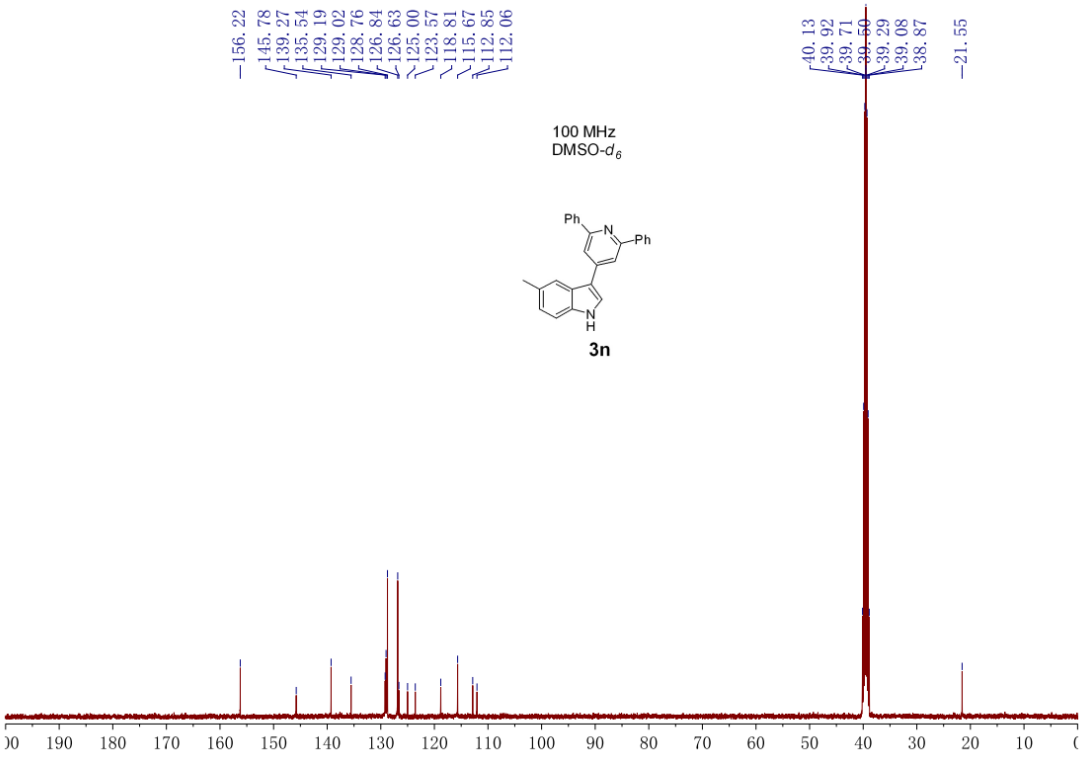
3.5
2.5
1.5
0.5
−0.5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139.27
135.54
129.19
129.02
128.76
126.84
126.63
125.00
123.57
118.81
115.67
112.85
112.06
40.13
39.92
39.71
39.50
39.29
39.08
38.87
21.55
100 MHz
DMSO-d_6
Ph
N
Ph
N
H
3n
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150
140
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120
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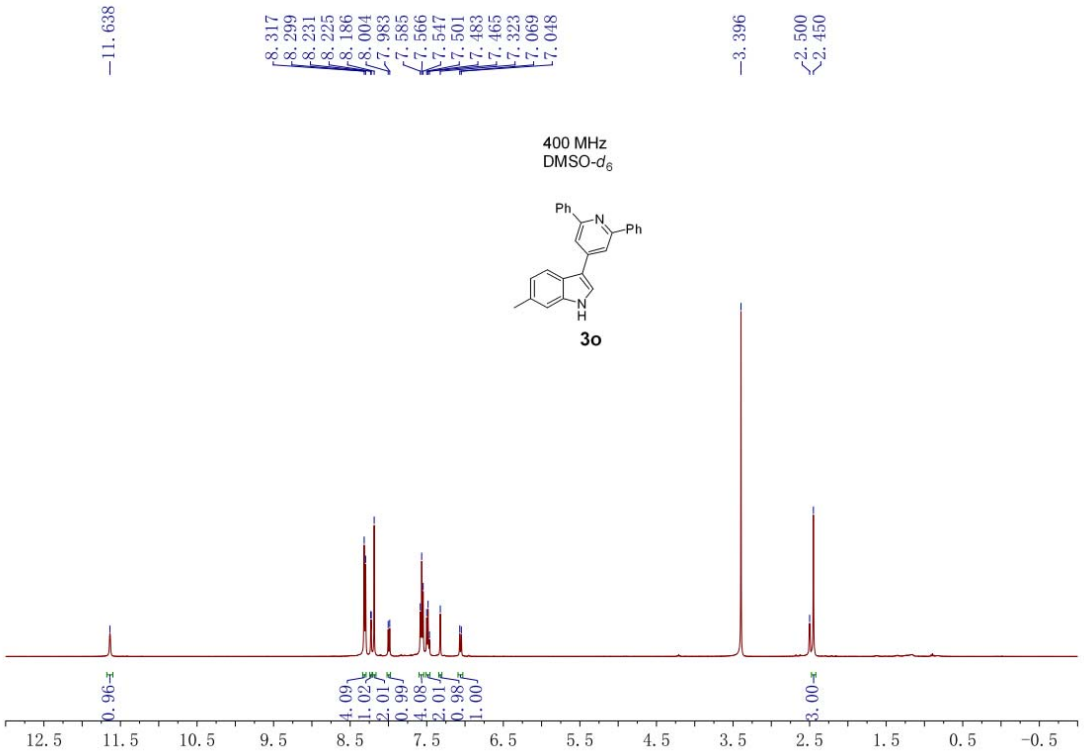
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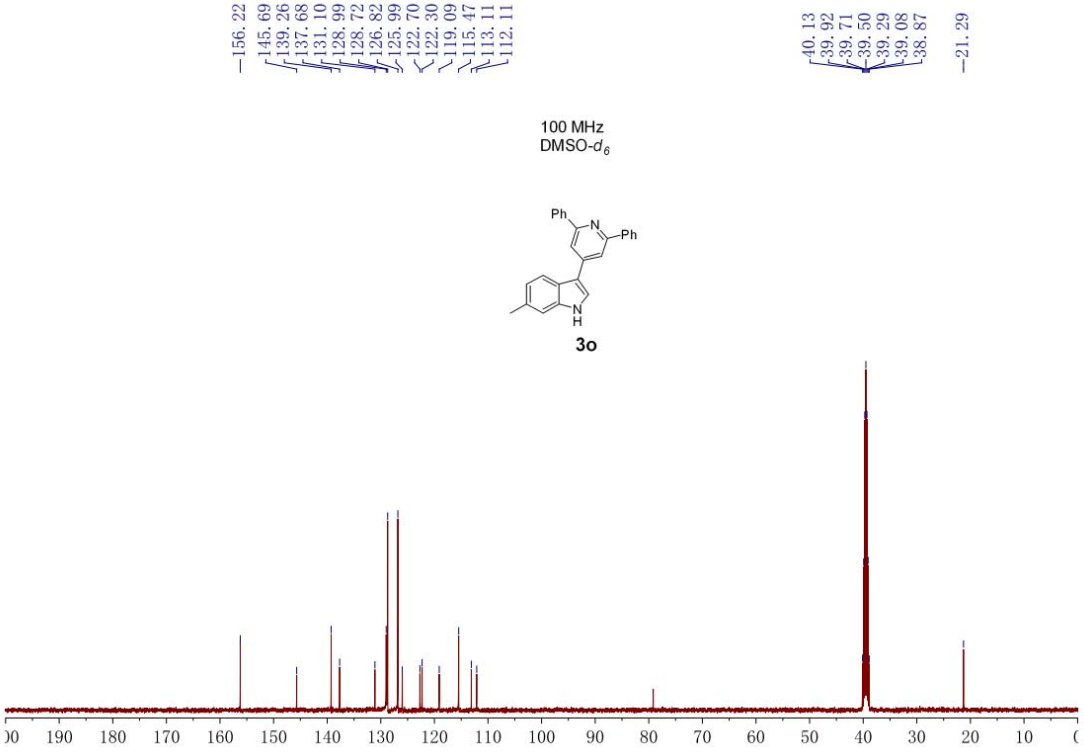
8.317
8.299
8.231
8.225
8.186
8.004
7.983
7.585
7.566
7.547
7.501
7.483
7.465
7.323
7.069
7.048
3.396
2.500
2.450
400 MHz
DMSO-d_6
Ph
N
Ph
N
H
3o
0.96
4.09
1.02
2.01
0.99
4.08
2.01
0.98
1.00
3.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5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128.99
128.72
126.82
125.99
122.70
122.30
119.09
115.47
113.11
112.11
40.13
39.92
39.71
39.50
39.29
39.08
38.87
21.29
100 MHz
DMSO-d_6
Ph
N
Ph
N
H
3o
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180
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160
150
140
130
120
110
100
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80
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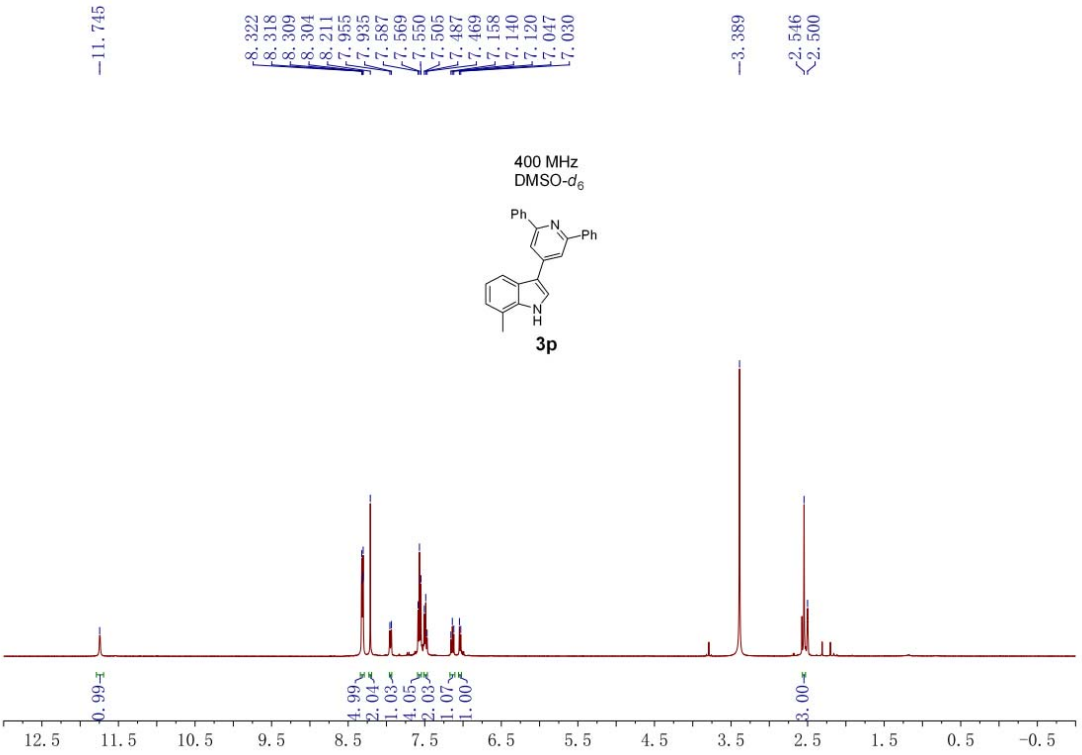
40
30
20
10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8.304
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7.955
7.935
7.587
7.569
7.550
7.505
7.487
7.469
7.158
7.140
7.120
7.047
7.030
3.389
2.546
2.500
400 MHz
DMSO-d_6
Ph
N
Ph
N
H
3p
0.99
4.99
2.04
1.03
4.05
2.03
1.07
1.00
3.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
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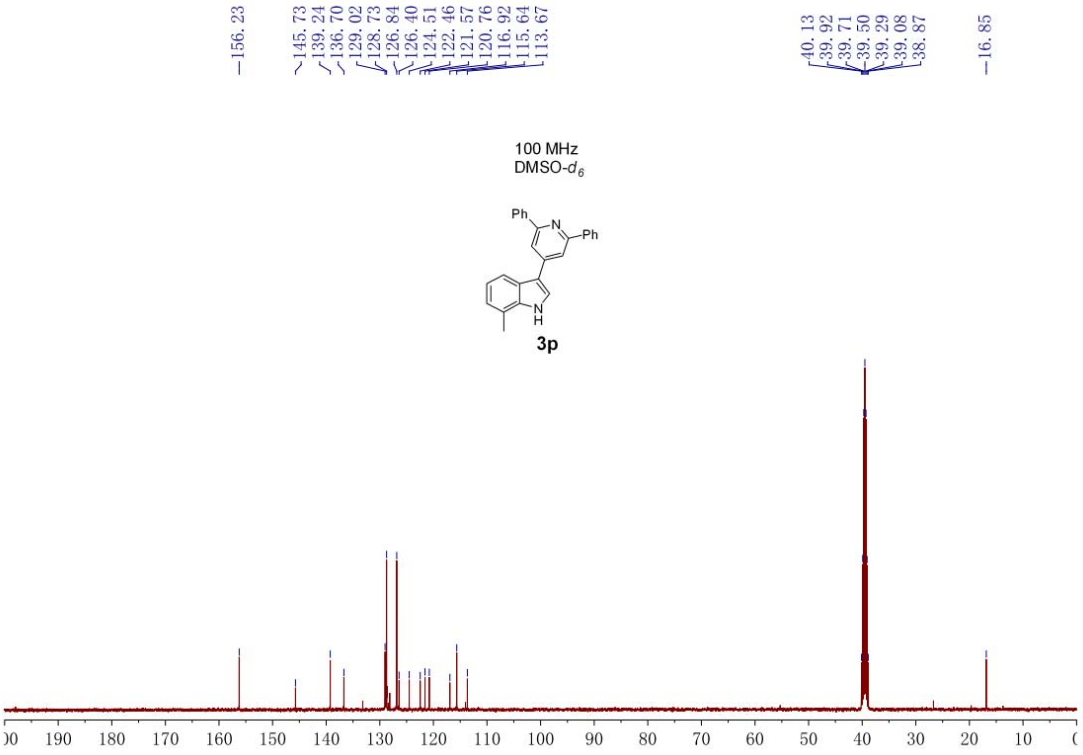
1.5
0.5
−0.5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126.84
126.40
124.51
122.46
121.57
120.76
116.92
115.64
113.67
40.13
39.92
39.71
39.50
39.29
39.08
38.87
16.85
100 MHz
DMSO-d_6
Ph
N
Ph
N
H
3p
190
180
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160
150
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130
120
110
100
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80
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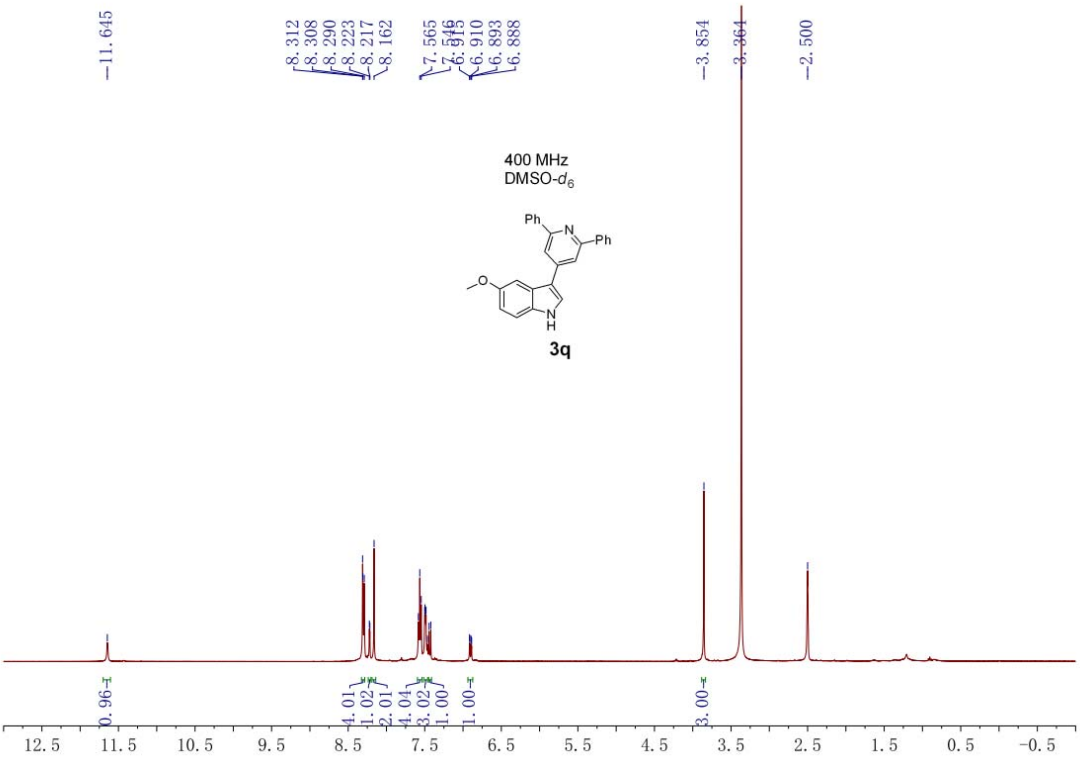
20
10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8.223
8.217
8.162
7.565
7.546
6.913
6.910
6.893
6.888
3.854
3.364
2.500
400 MHz
DMSO-d_6
Ph
N
Ph
O
N
H
3q
0.96
4.01
1.02
2.01
4.04
3.02
1.00
1.00
3.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
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0.5
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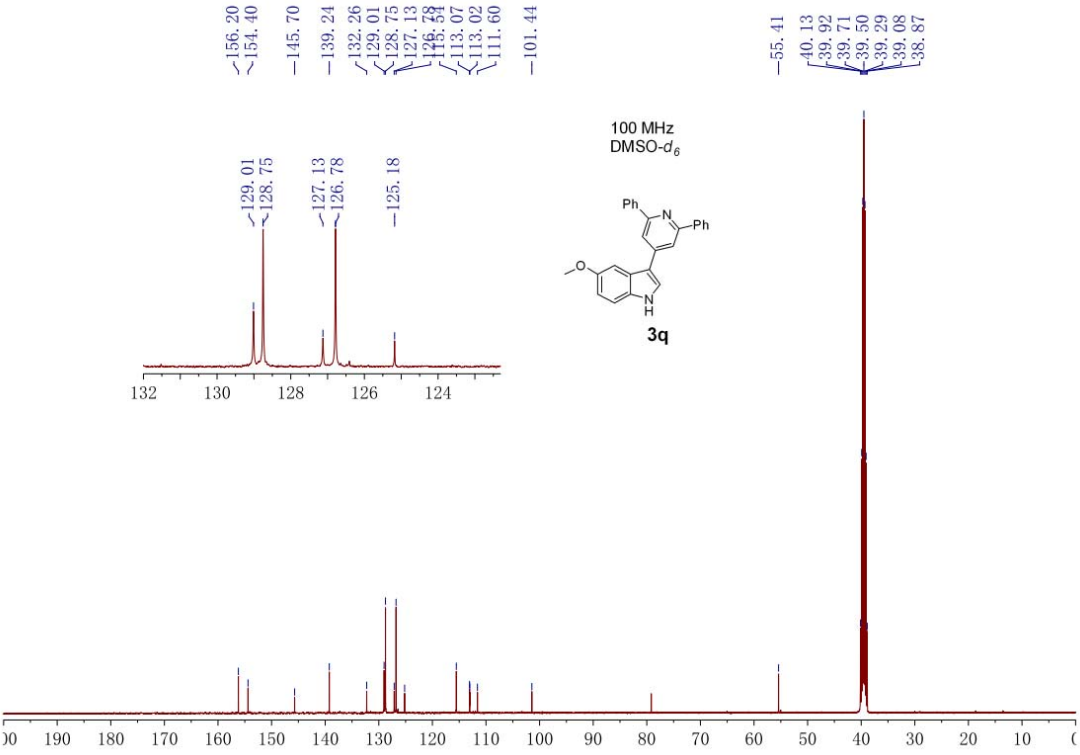
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154.40
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139.24
132.26
129.01
128.75
127.13
126.78
125.54
125.18
113.07
113.02
111.60
101.44
55.41
40.13
39.92
39.71
39.50
39.29
39.08
38.87
129.01
128.75
127.13
126.78
125.18
132
130
128
126
124
100 MHz
DMSO-d_6
Ph
N
Ph
O
N
H
3q
190
180
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120
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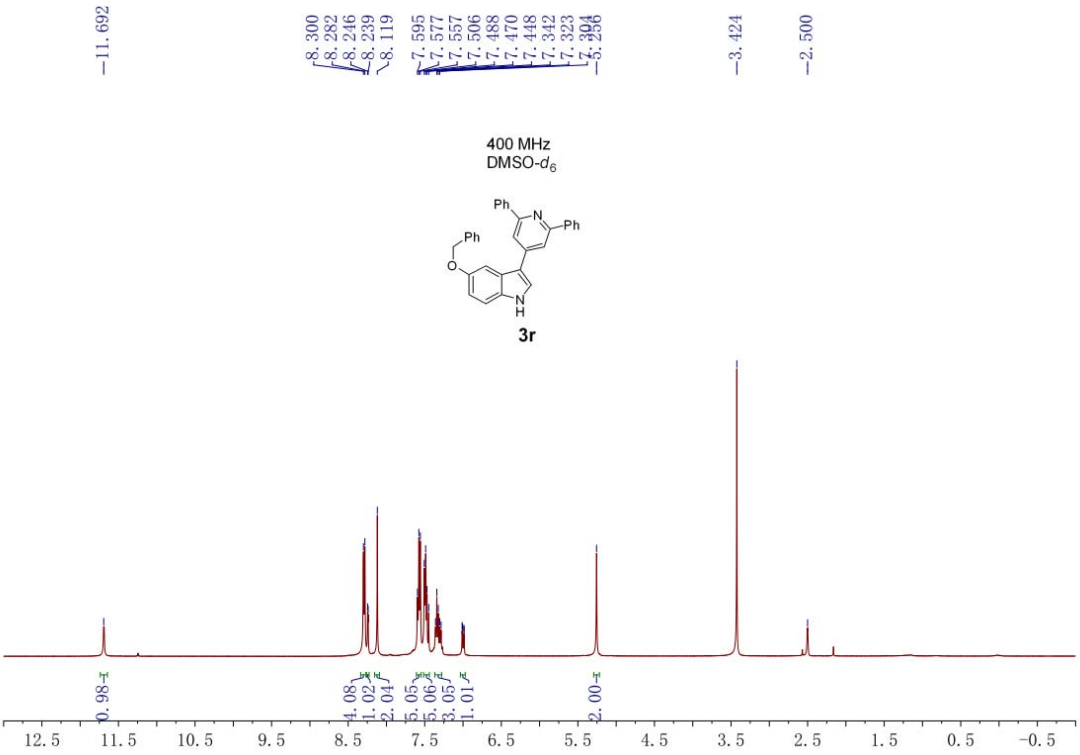
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8.239
8.119
7.595
7.577
7.557
7.506
7.488
7.470
7.448
7.342
7.323
5.756
3.424
2.500
400 MHz
DMSO-d_6
3r
0.98
4.08
1.02
2.04
5.05
5.06
3.05
1.01
2.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
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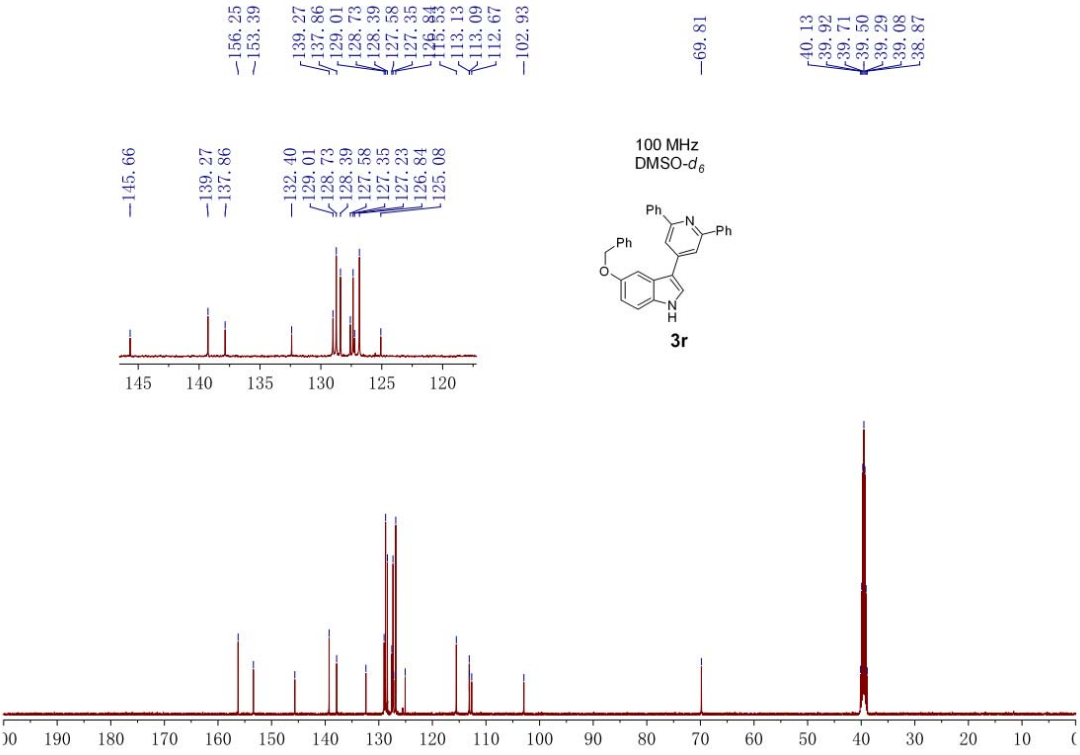
2.5
1.5
0.5
−0.5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127.58
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125.53
113.13
113.09
112.67
102.93
69.81
40.13
39.92
39.71
39.50
39.29
39.08
38.87
145.66
139.27
137.86
132.40
129.01
128.73
128.39
127.58
127.35
127.23
126.84
125.08
100 MHz
DMSO-d_6
3r
145
140
135
130
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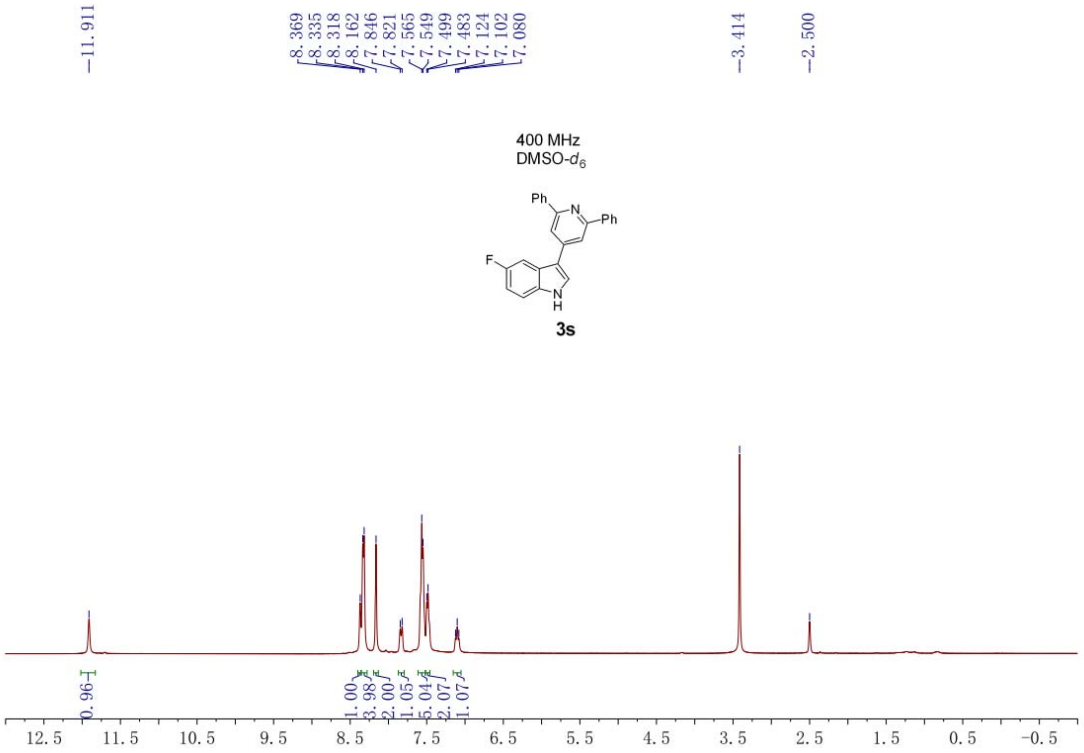
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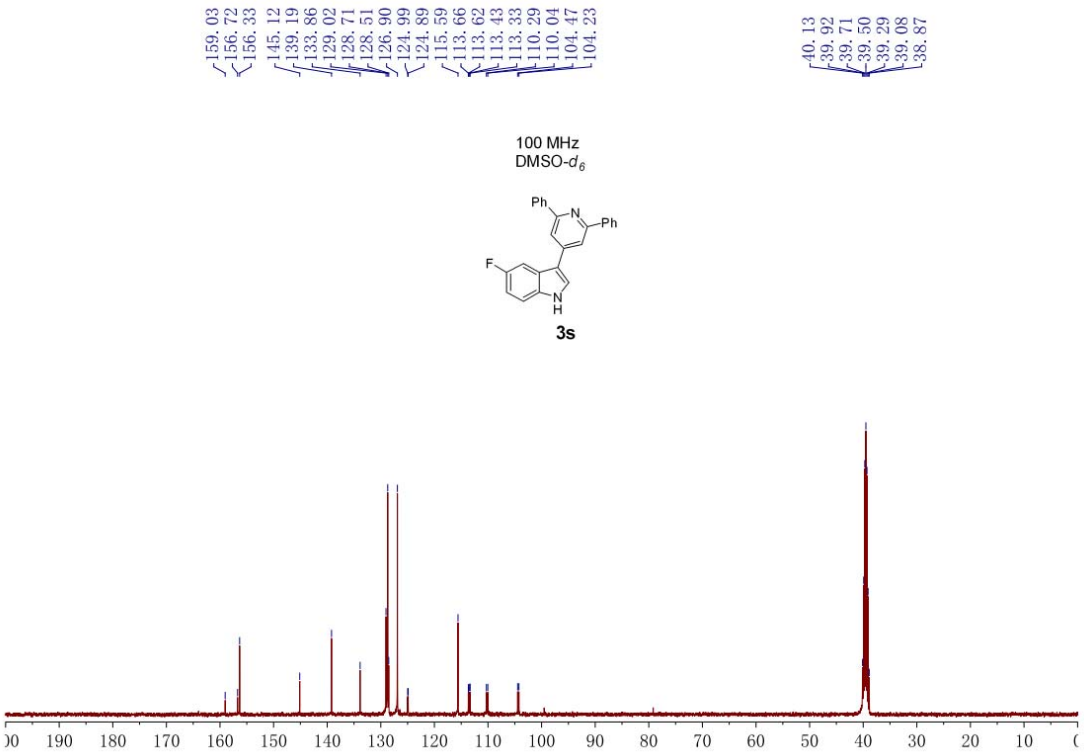
7.846
7.821
7.565
7.549
7.499
7.483
7.124
7.102
7.080
3.414
2.500
400 MHz
DMSO-d_6
Ph
N
Ph
F
N
H
3s
0.96
1.00
3.98
2.00
1.05
6.04
2.07
1.07
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5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133.86
129.02
128.71
128.51
126.90
124.99
124.89
115.59
113.66
113.62
113.43
113.33
110.29
110.04
104.47
104.23
40.13
39.92
39.71
39.50
39.29
39.08
38.87
100 MHz
DMSO-d_6
Ph
N
Ph
F
N
H
3s
190
180
170
160
150
140
130
120
110
100
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80
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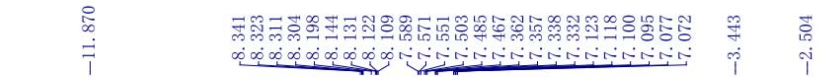
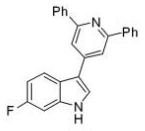
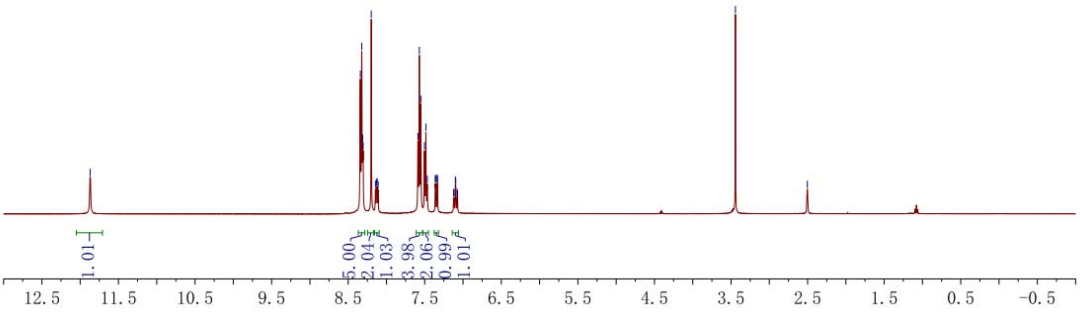
40
30
20
10

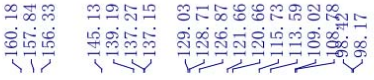


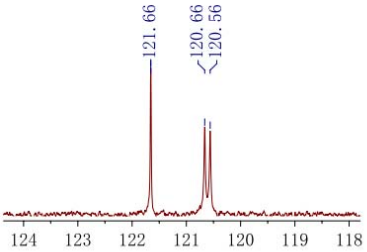
400 MHz
DMSO-d_6



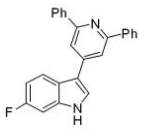
3t



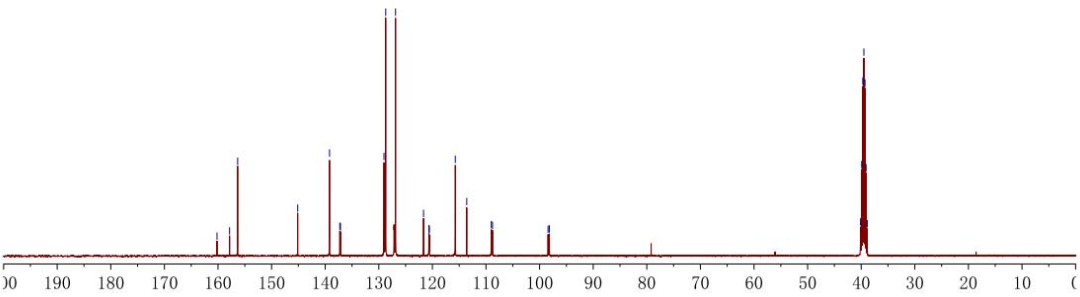


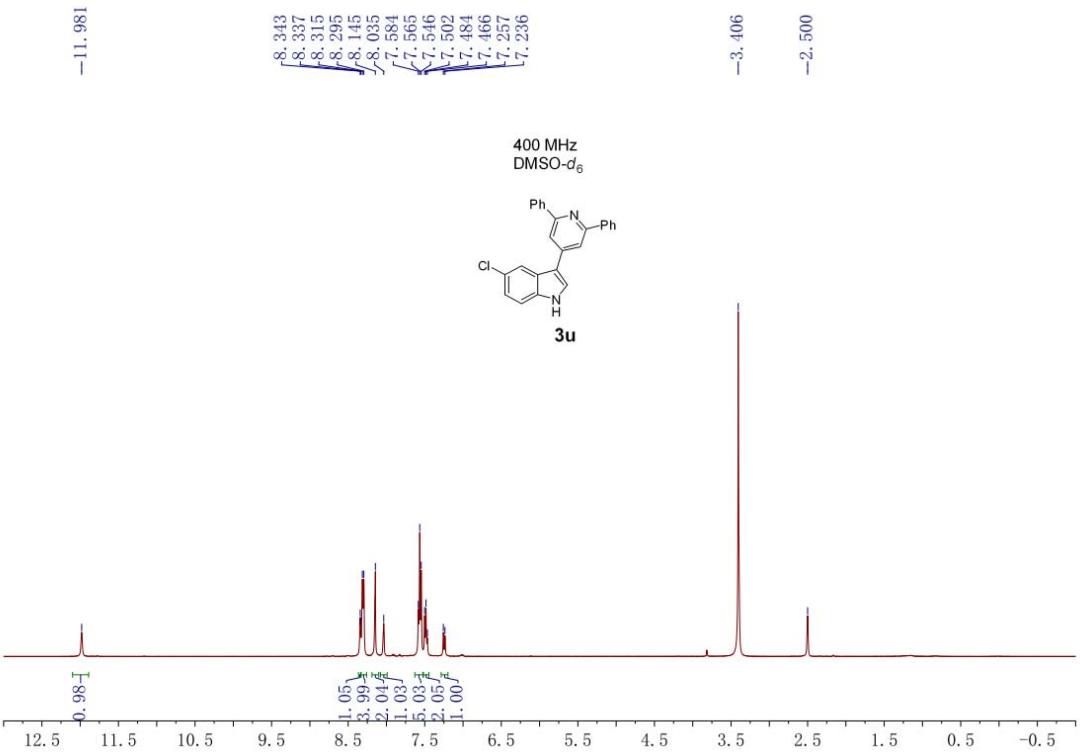


100 MHz
DMSO-d_6



3t

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8.343
8.337
8.315
8.295
8.145
8.035
7.584
7.565
7.546
7.502
7.484
7.466
7.257
7.236
3.406
2.500
400 MHz
DMSO-d_6
Ph
N
Ph
Cl
N
H
3u
0.98
1.05
3.99
2.04
1.03
5.03
2.05
1.00
12.5
11.5
10.5
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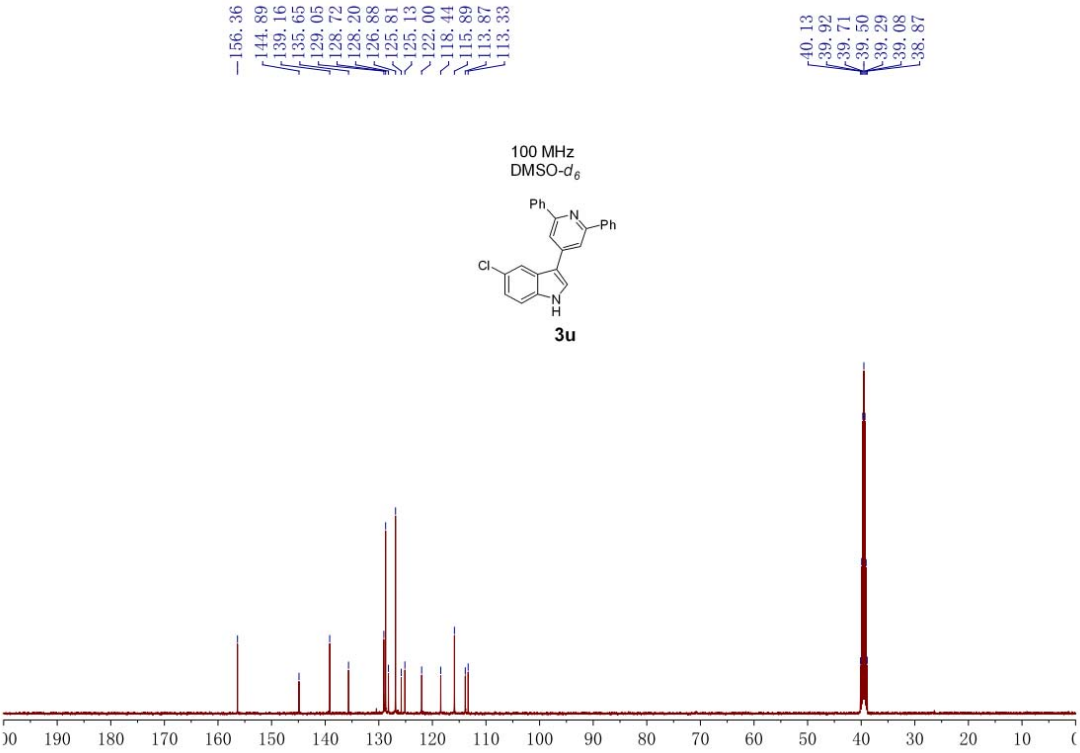
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5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135.65
129.05
128.72
128.20
126.88
125.81
125.13
122.00
118.44
115.89
113.87
113.33
40.13
39.92
39.71
39.50
39.29
39.08
38.87
100 MHz
DMSO-d_6
Ph
N
Ph
Cl
N
H
3u
190
180
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140
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120
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80
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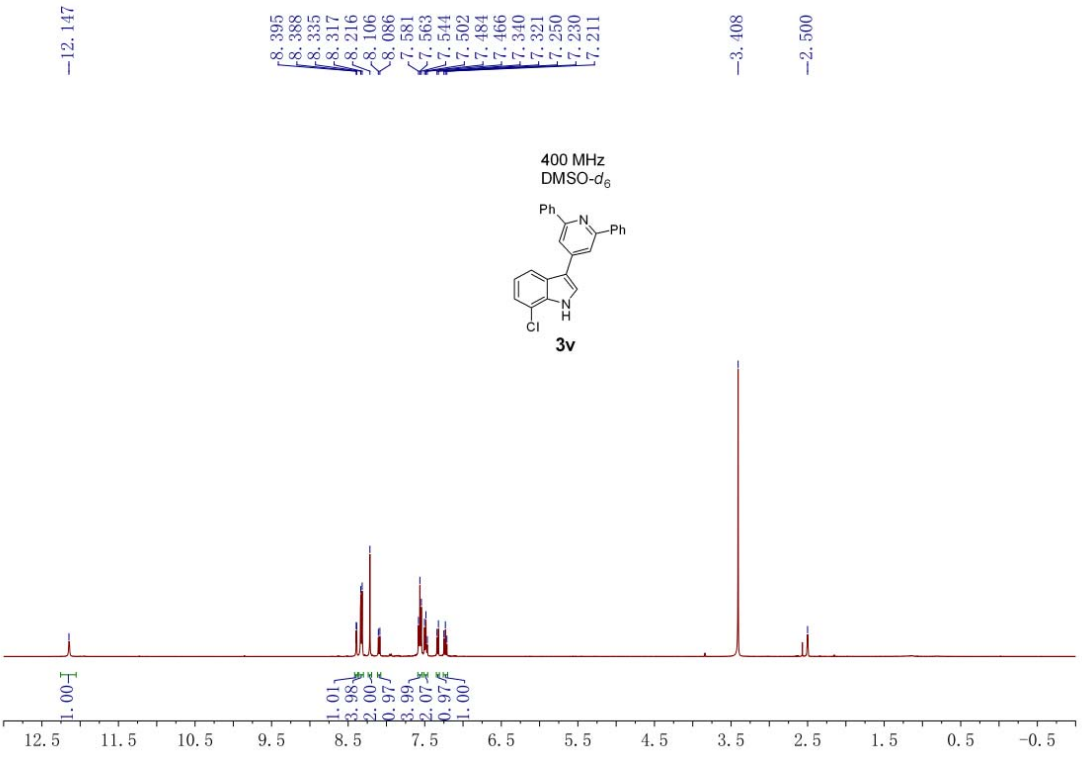
10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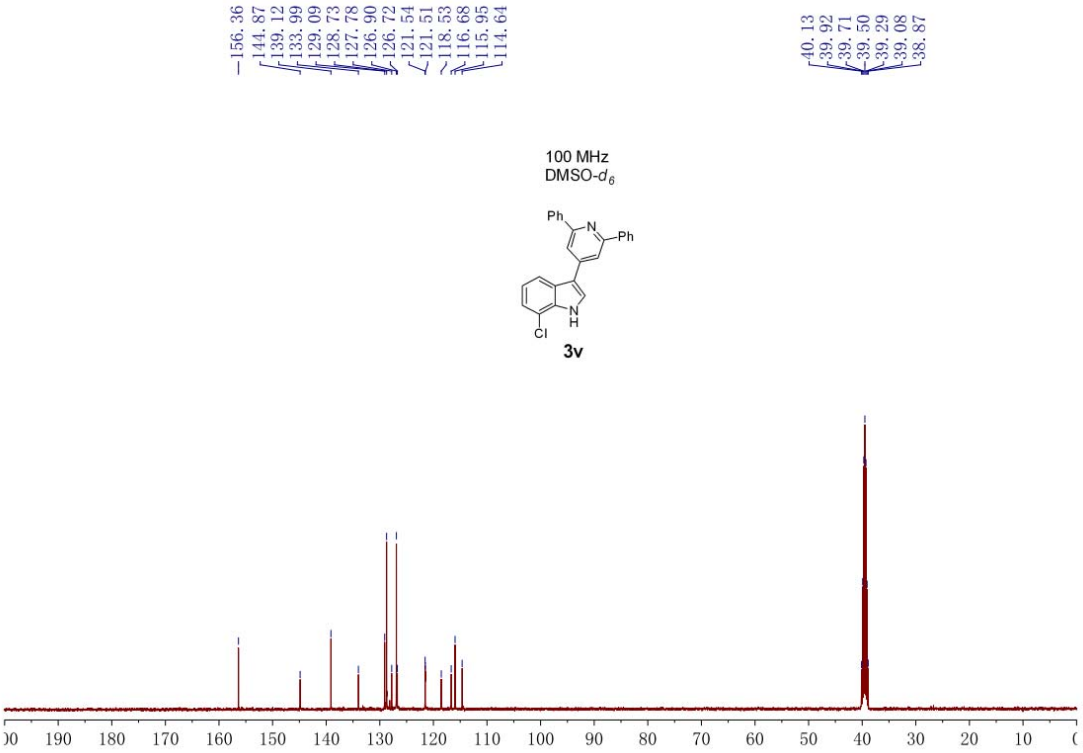
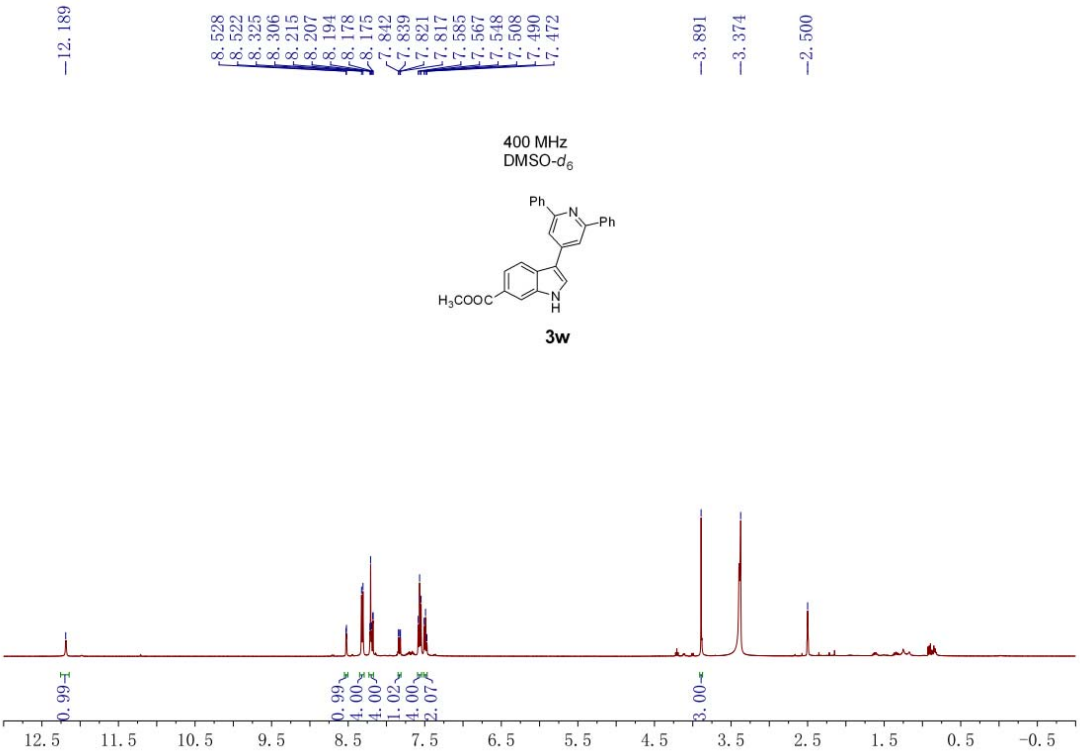
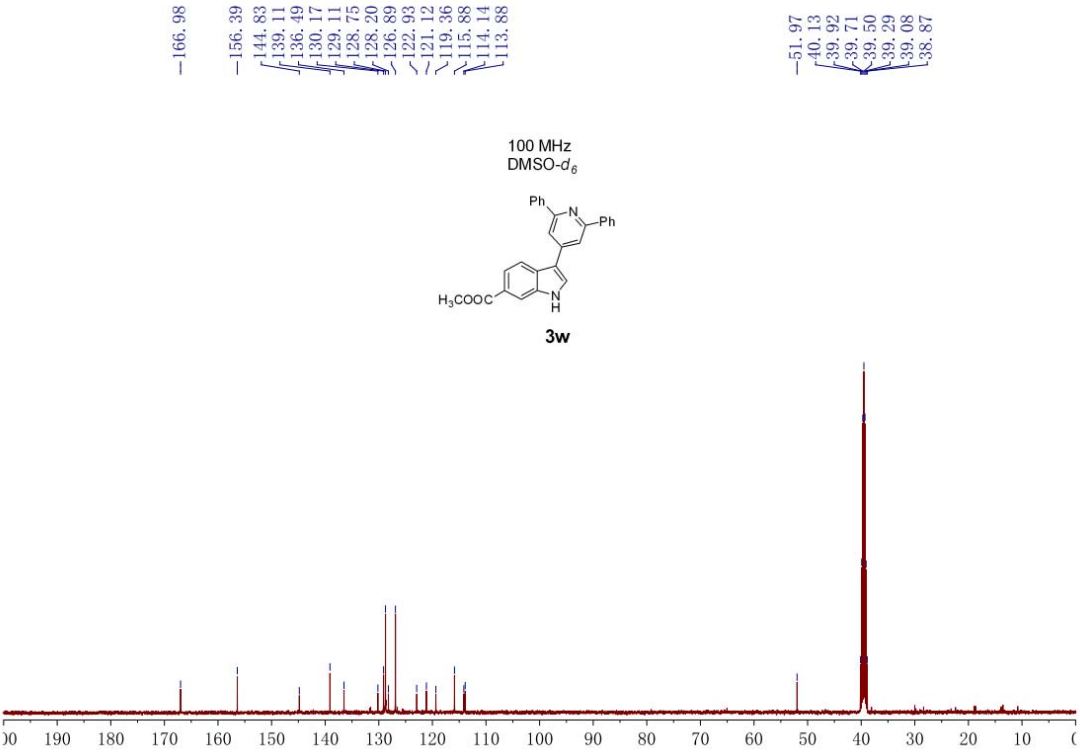
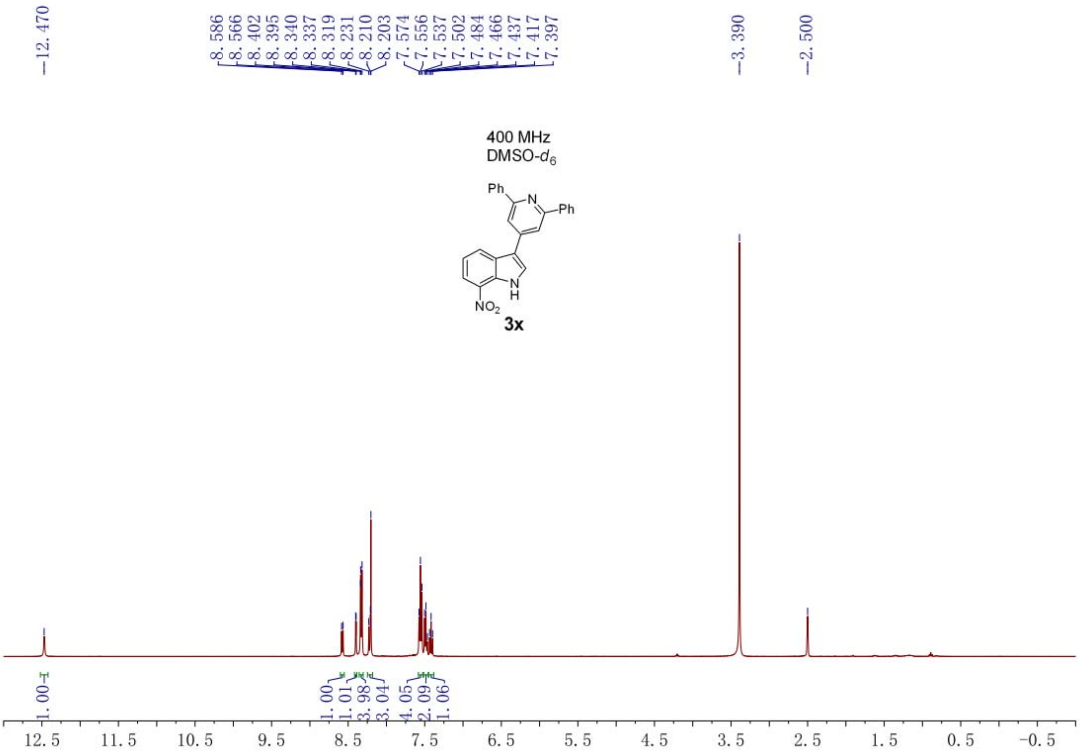
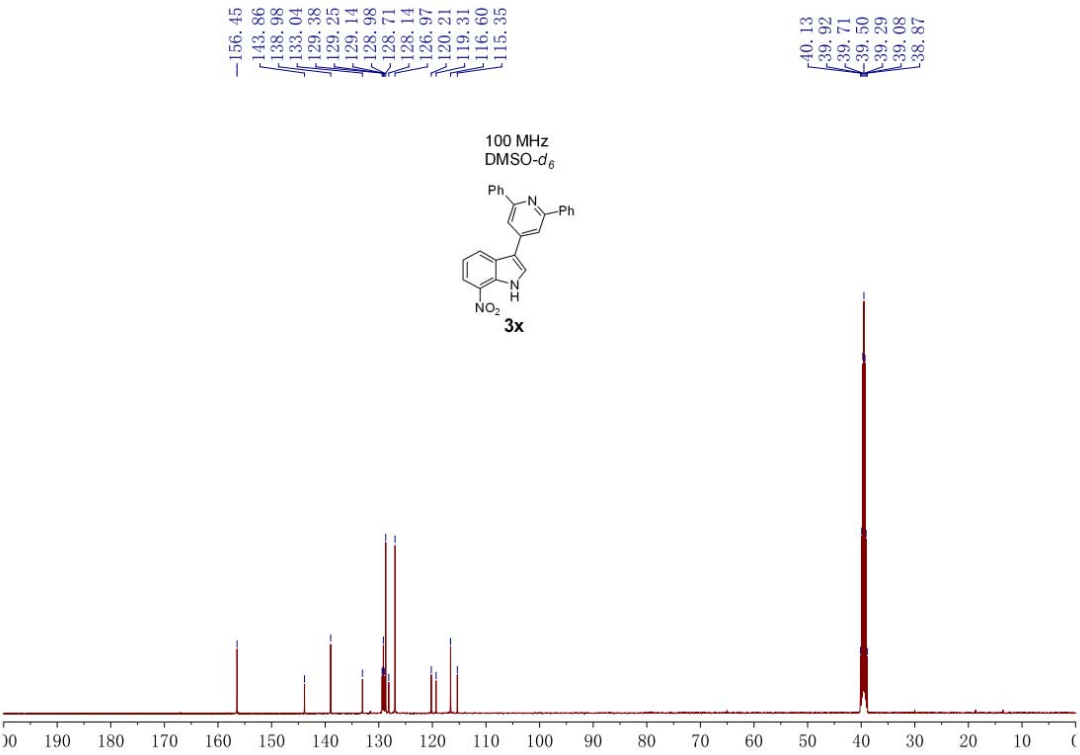
8.335
8.317
8.216
8.106
8.086
7.581
7.563
7.544
7.502
7.484
7.466
7.340
7.321
7.250
7.230
7.211
3.408
2.500
400 MHz
DMSO-d_6
Ph
N
Ph
N
H
Cl
3v
1.00
1.01
3.98
2.00
0.97
3.99
2.07
0.97
1.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5

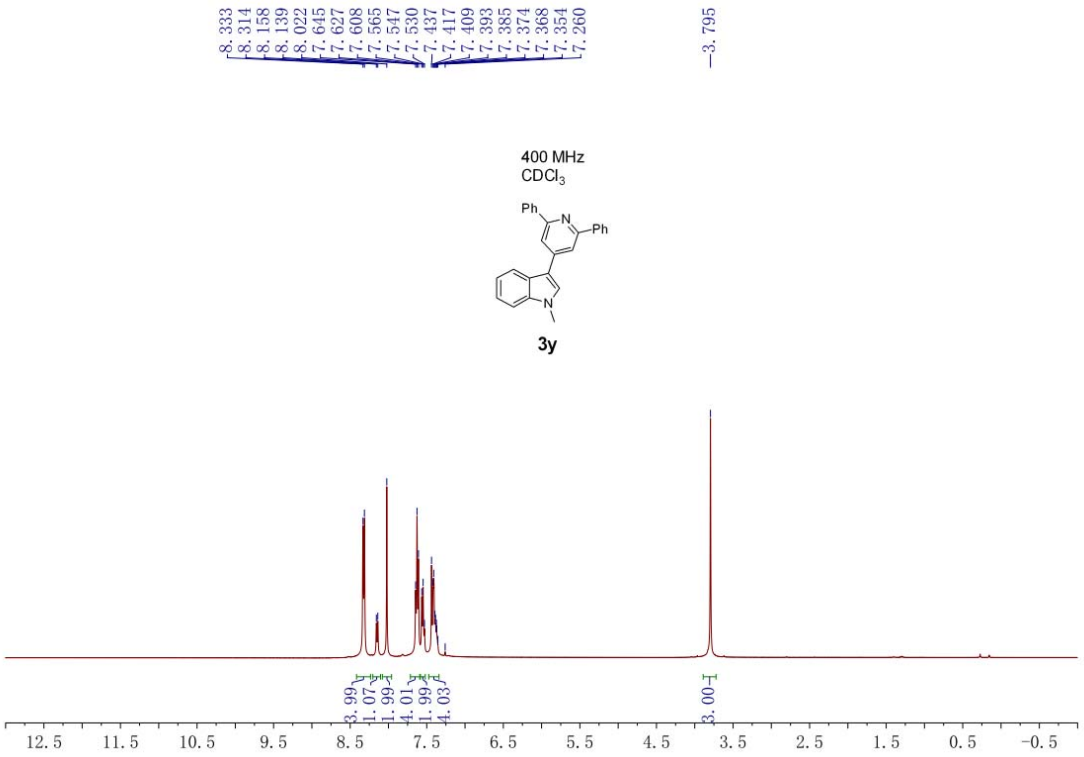

156.36
144.87
139.12
133.99
129.09
128.73
127.78
126.90
126.72
121.54
121.51
118.53
116.68
115.95
114.64
40.13
39.92
39.71
39.50
39.29
39.08
38.87
100 MHz
DMSO-d_6
Ph
N
Ph
N
H
Cl
3v
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

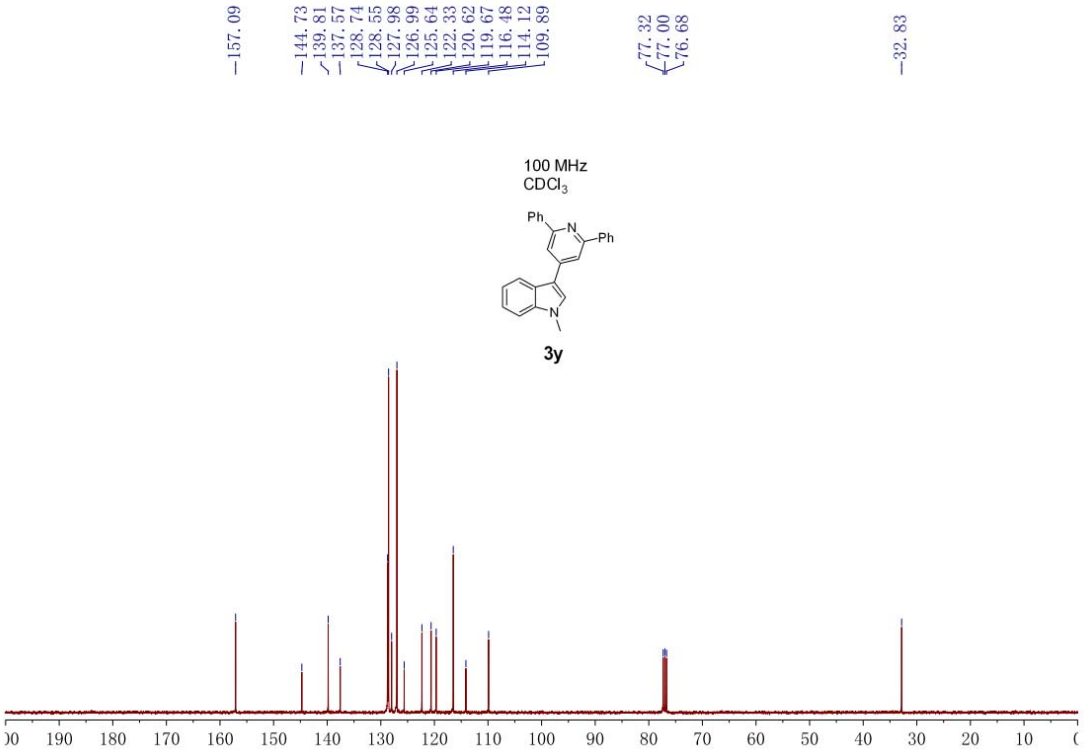

12.189
8.528
8.522
8.325
8.306
8.215
8.207
8.194
8.178
8.175
7.842
7.839
7.821
7.817
7.585
7.567
7.548
7.508
7.490
7.472
3.891
3.374
2.500
400 MHz
DMSO-d_6
Ph
N
Ph
H_3COOC
N
H
3w
0.99
4.00
4.00
1.02
4.00
2.07
3.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5

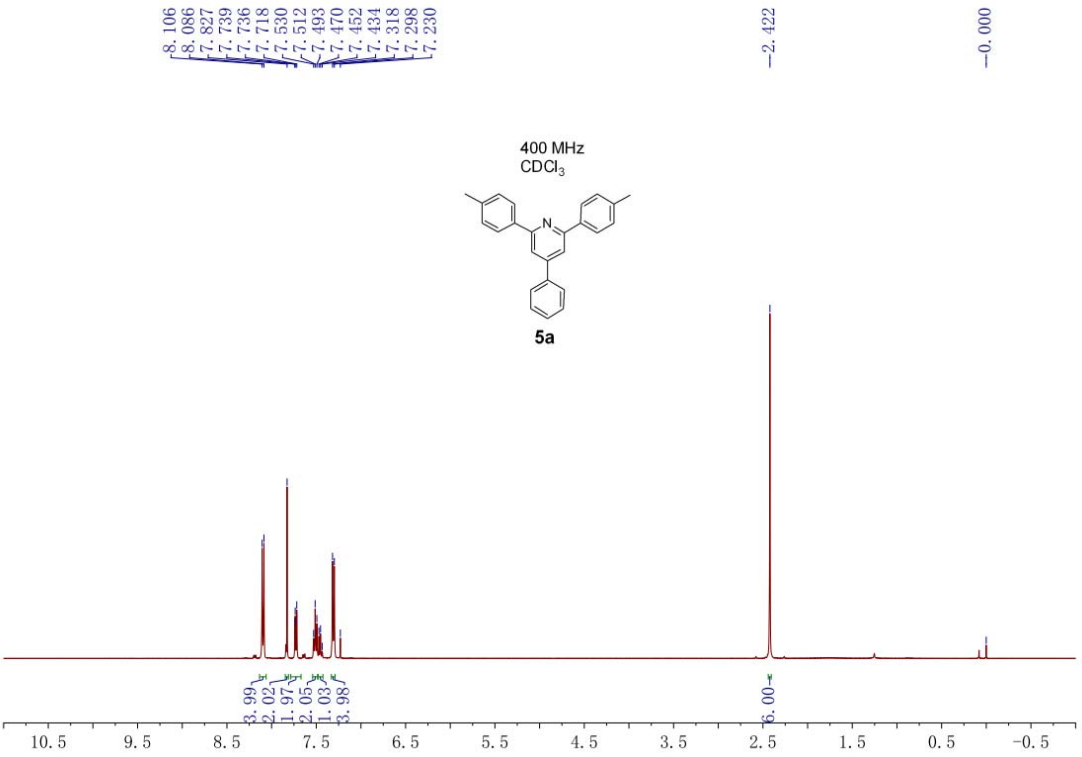

166.98
156.39
144.83
139.11
136.49
130.17
129.11
128.75
128.20
126.89
122.93
121.12
119.36
115.88
114.14
113.88
51.97
40.13
39.92
39.71
39.50
39.29
39.08
38.87
100 MHz
DMSO-d_6
Ph
N
Ph
H_3COOC
N
H
3w
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

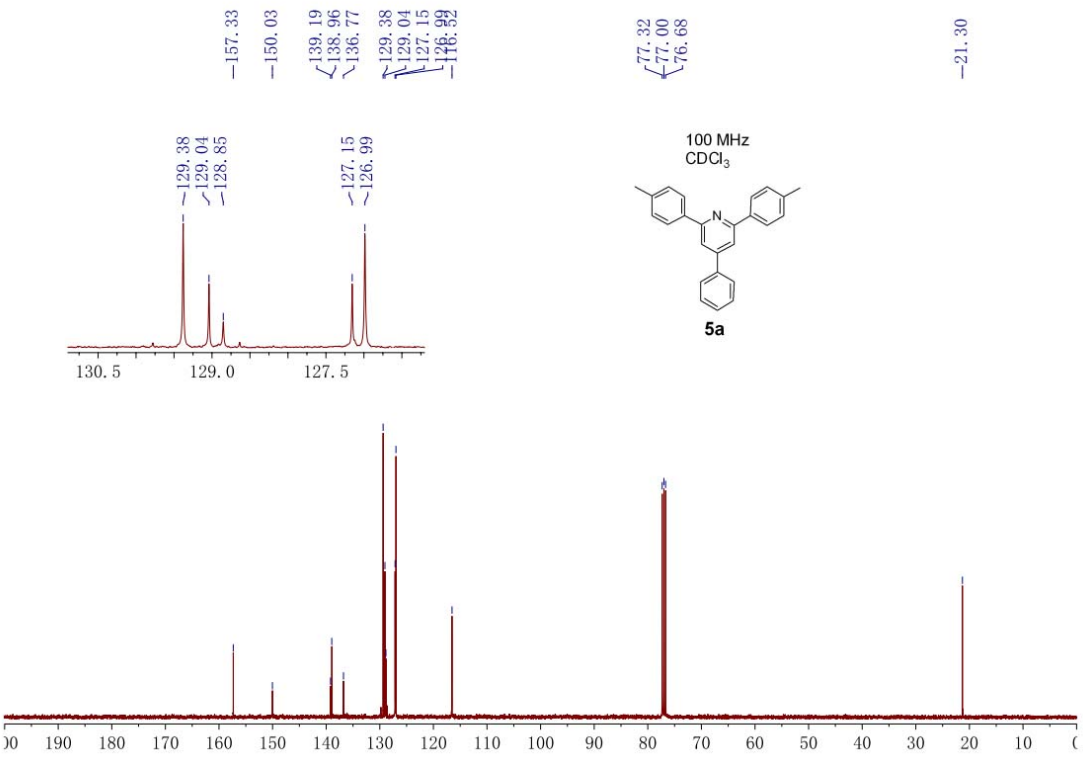

12.470
8.586
8.566
8.402
8.395
8.340
8.337
8.319
8.231
8.210
8.203
7.574
7.556
7.537
7.502
7.484
7.466
7.437
7.417
7.397
3.390
2.500
400 MHz
DMSO-d_6
Ph
N
Ph
N
H
NO2
3x
1.00
1.00
1.01
3.98
3.04
4.05
2.09
1.06
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5

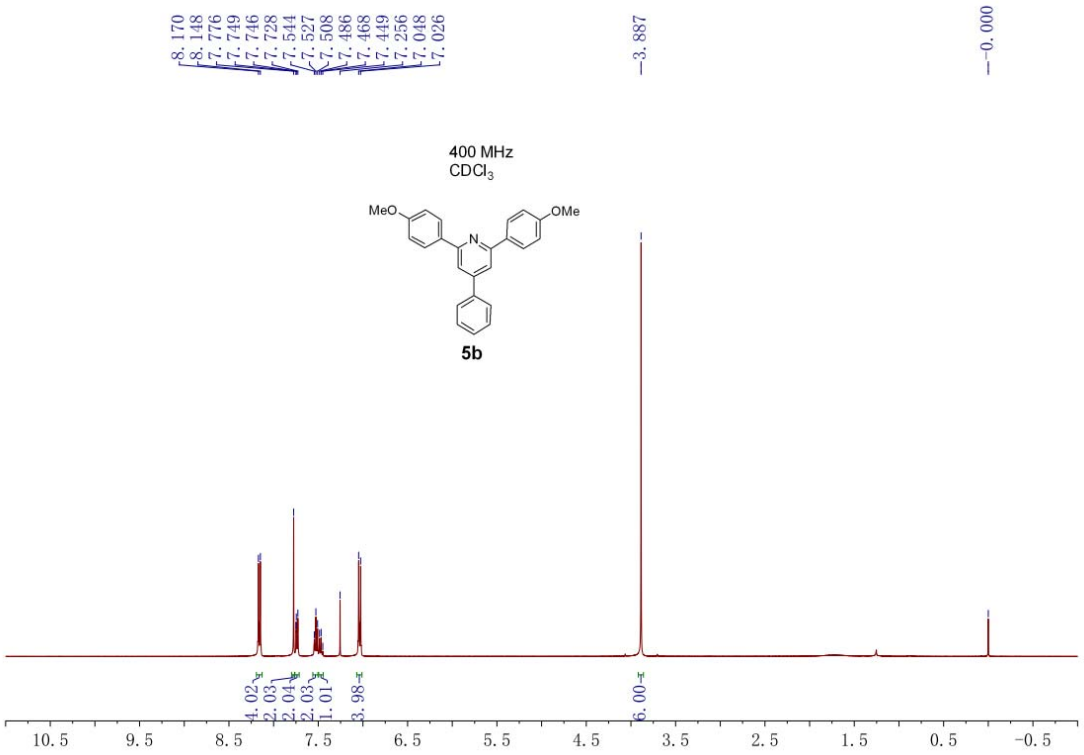

156.45
143.86
138.98
133.04
129.38
129.25
129.14
128.98
128.71
128.14
126.97
120.21
119.31
116.60
115.35
40.13
39.92
39.71
39.50
39.29
39.08
38.87
100 MHz
DMSO-d_6
Ph
N
Ph
N
H
NO2
3x
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

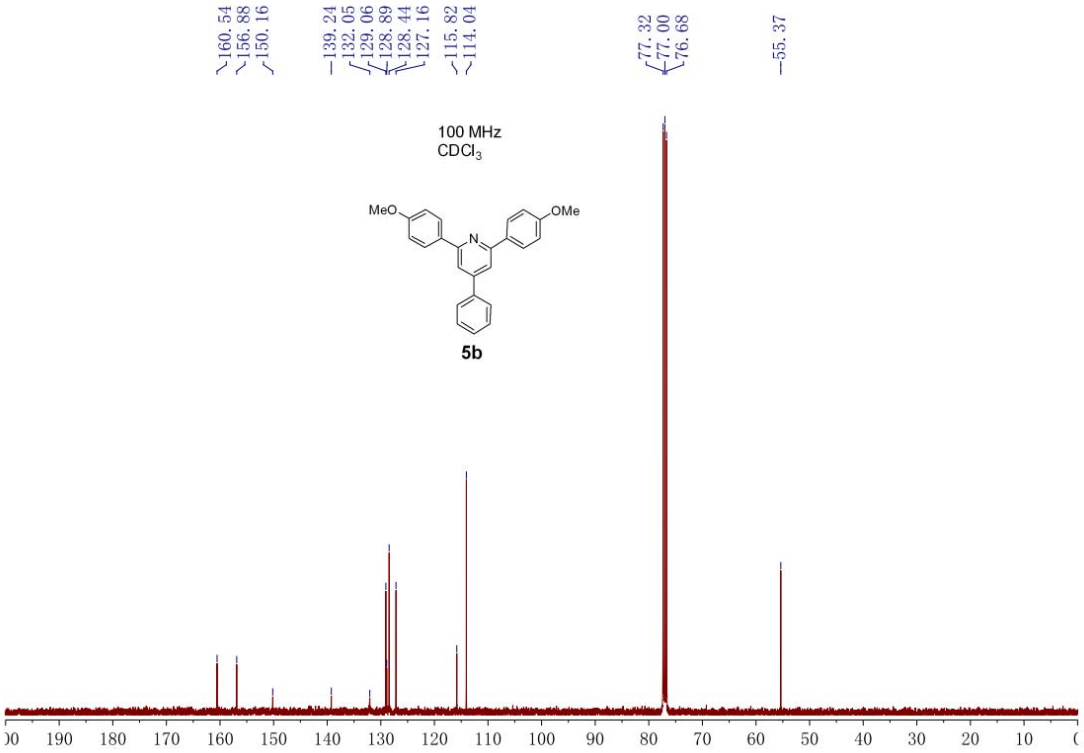

8.333
8.314
8.158
8.139
8.022
7.645
7.627
7.608
7.565
7.547
7.530
7.437
7.417
7.409
7.393
7.385
7.374
7.368
7.354
7.260
3.795
400 MHz
CDCl3
Ph
N
Ph
N
3y
3.99
1.07
1.99
4.01
1.99
4.03
3.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

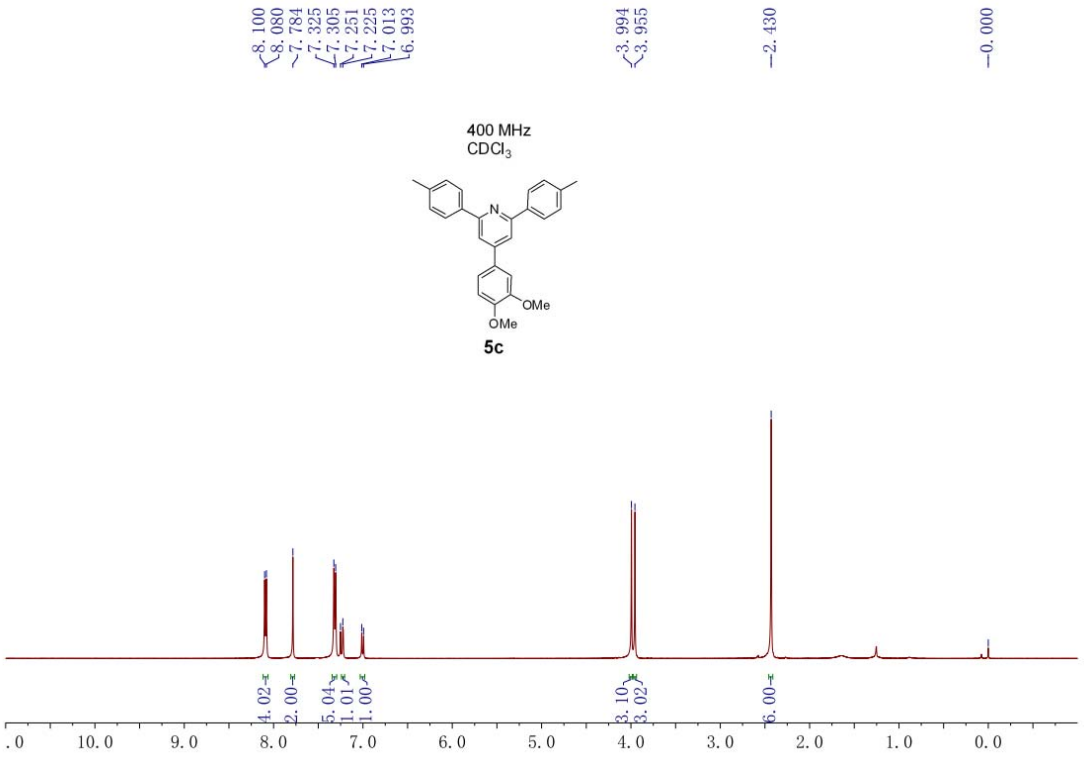

157.09
144.73
139.81
137.57
128.74
128.55
127.98
126.99
125.64
122.33
120.62
119.67
116.48
114.12
109.89
77.32
77.00
76.68
32.83
100 MHz
CDCl3
Ph
N
Ph
N
3y
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

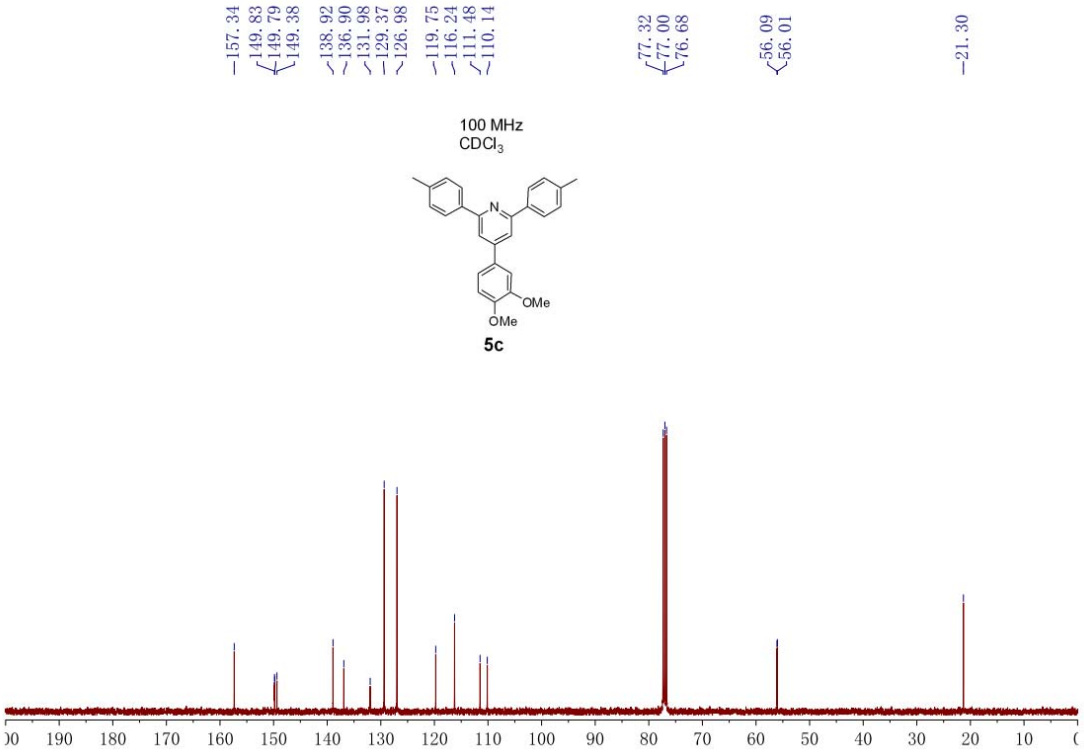

8.106
8.086
7.827
7.739
7.736
7.718
7.530
7.512
7.493
7.470
7.452
7.434
7.318
7.298
7.230
2.422
0.000
400 MHz
CDCl3
5a
3.99
2.02
1.97
2.05
1.03
3.98
6.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

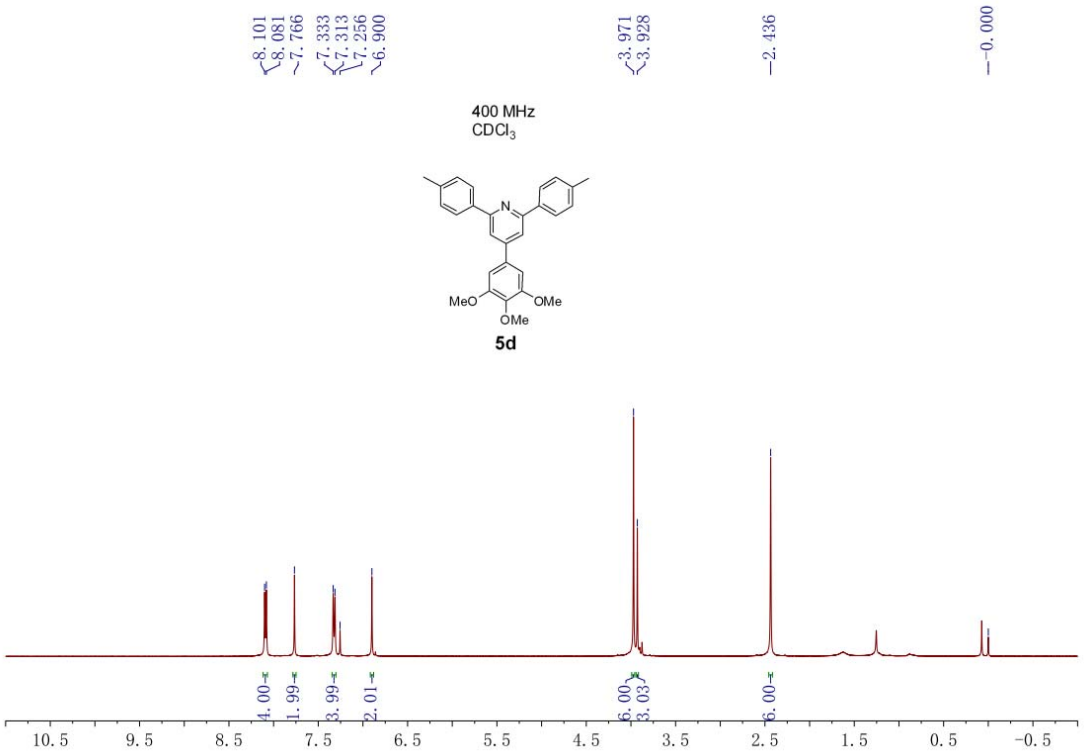

157.33
150.03
139.19
138.96
136.77
129.38
129.04
127.15
126.99
126.52
77.32
77.00
76.68
21.30
129.38
129.04
128.85
127.15
126.99
130.5
129.0
127.5
100 MHz
CDCl3
5a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

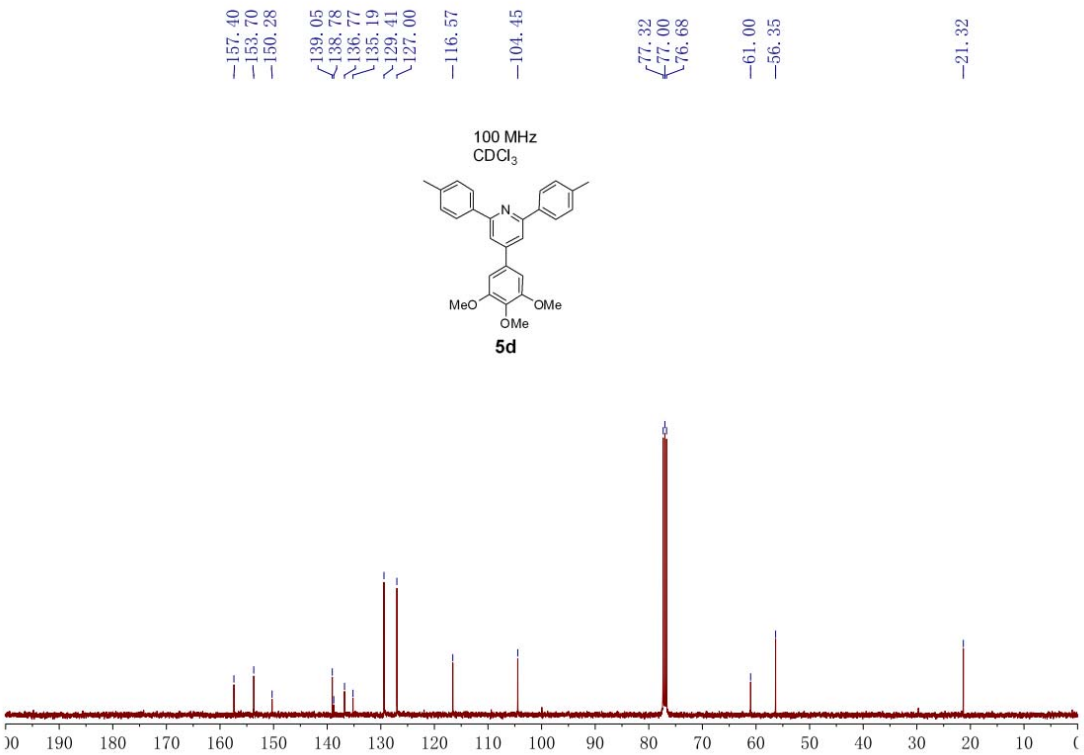

8.170
8.148
7.776
7.749
7.746
7.728
7.544
7.527
7.508
7.486
7.468
7.449
7.256
7.048
7.026
3.887
0.000
400 MHz
CDCl3
MeO
OMe
N
5b
4.02
2.03
2.04
2.03
1.01
3.98
6.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

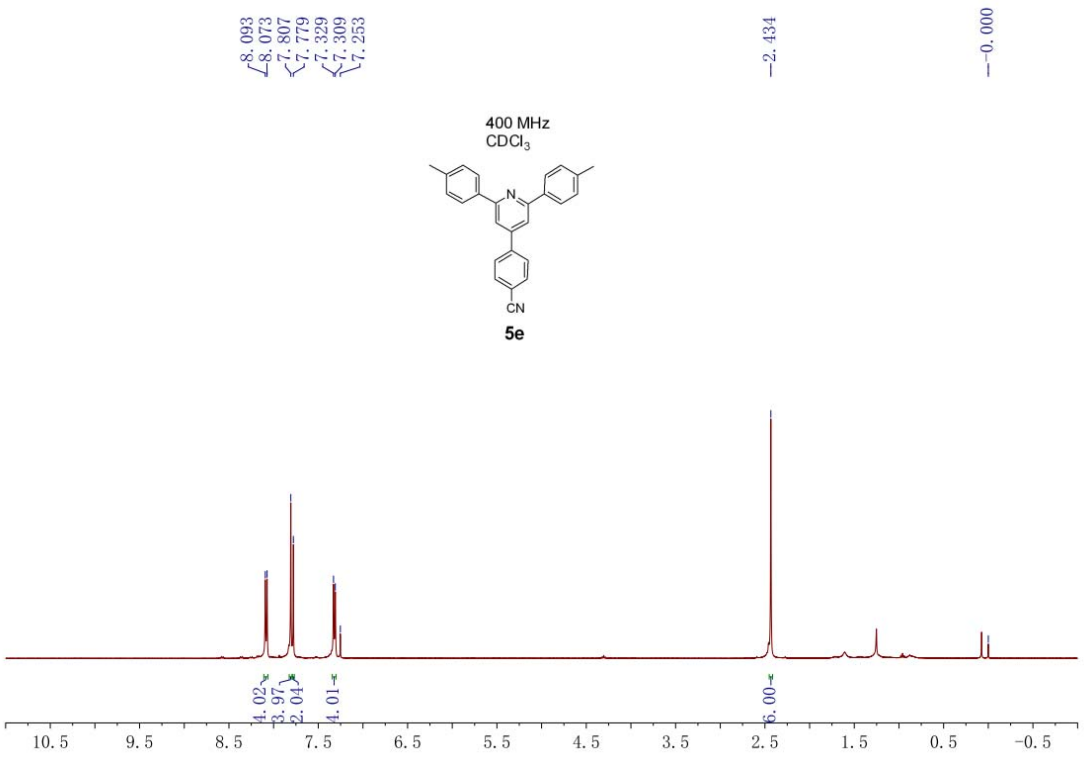

160.54
156.88
150.16
139.24
132.05
129.06
128.89
128.44
127.16
115.82
114.04
77.32
77.00
76.68
55.37
100 MHz
CDCl3
MeO
OMe
N
5b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

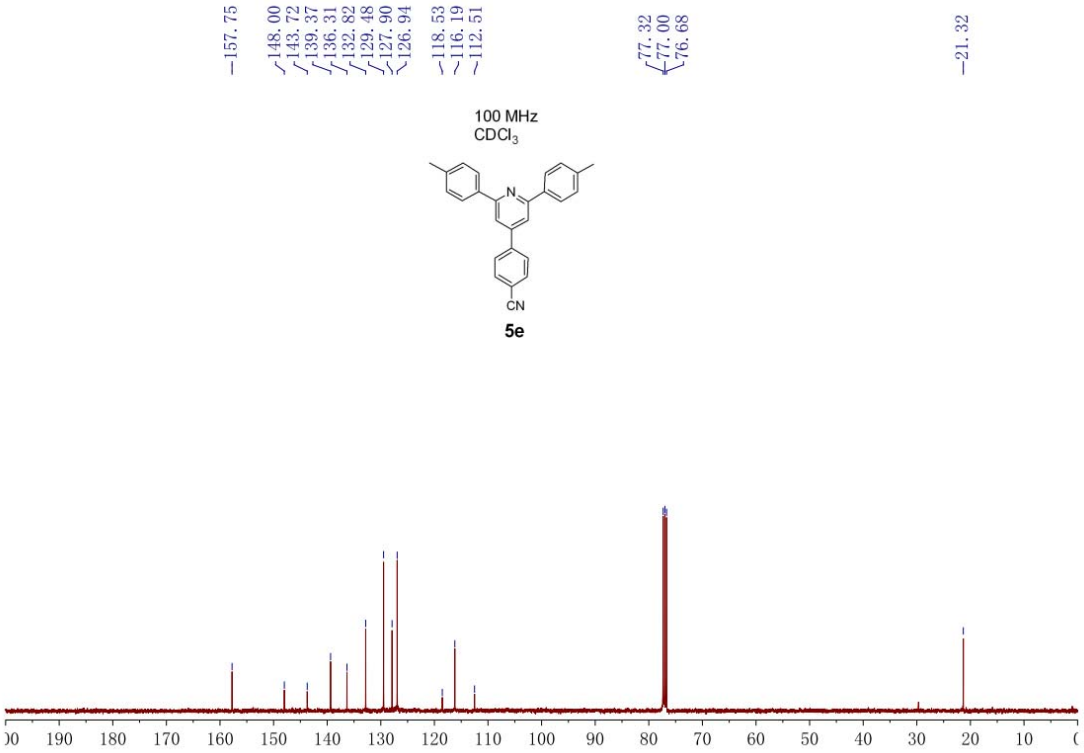

8.100
8.080
7.784
7.325
7.305
7.251
7.225
7.013
6.993
3.994
3.955
2.430
0.000
400 MHz
CDCl3
OMe
OMe
5c
4.02
2.00
5.04
1.01
1.00
3.10
3.02
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

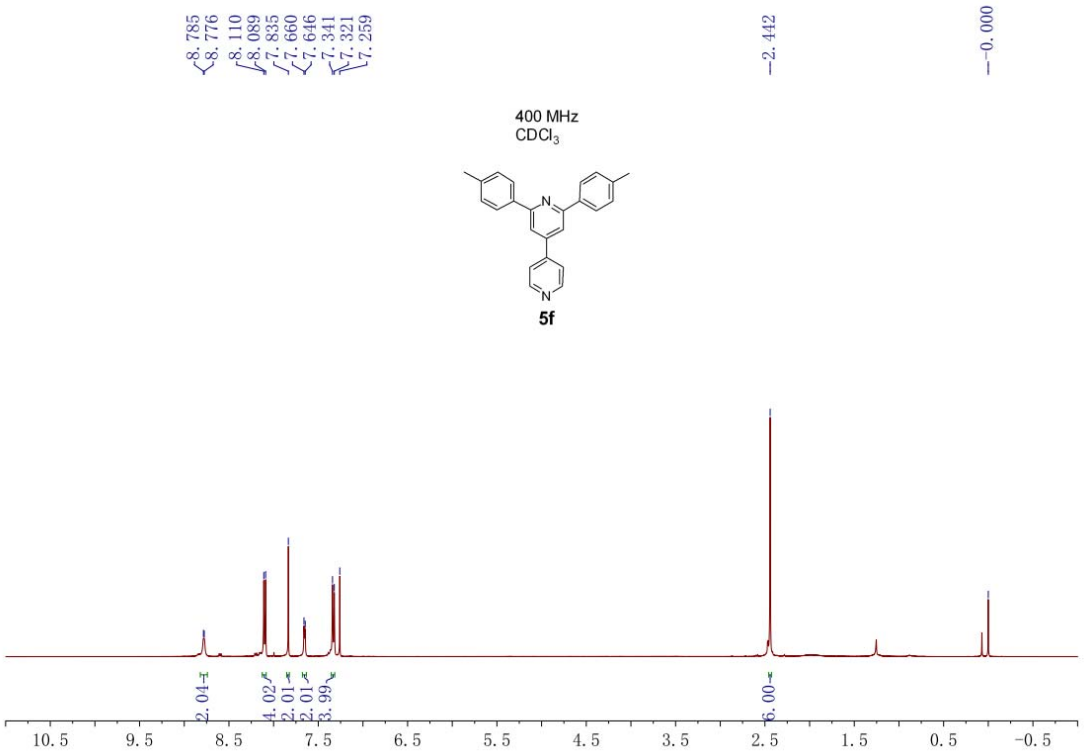

157.34
149.83
149.79
149.38
138.92
136.90
131.98
129.37
126.98
119.75
116.24
111.48
110.14
77.32
77.00
76.68
56.09
56.01
21.30
100 MHz
CDCl3
OMe
OMe
5c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

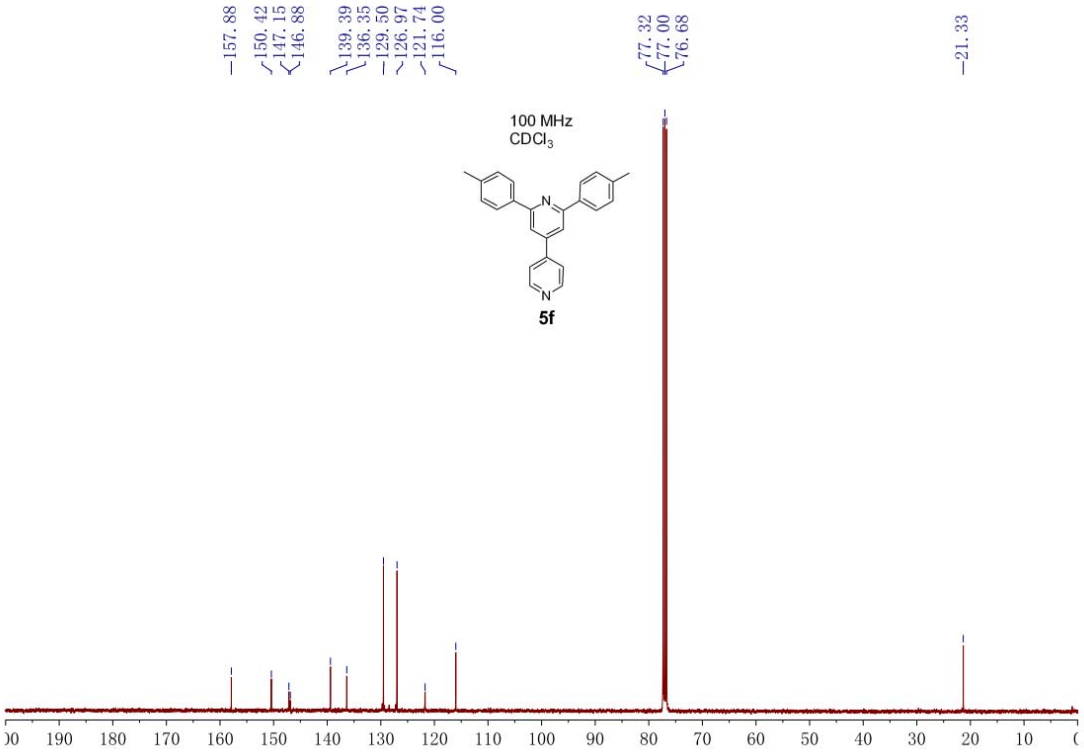

8.101
8.081
7.766
7.333
7.313
7.256
6.900
3.971
3.928
2.436
0.000
400 MHz
CDCl3
MeO
OMe
OMe
5d
4.00
1.99
3.99
2.01
6.00
3.03
6.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

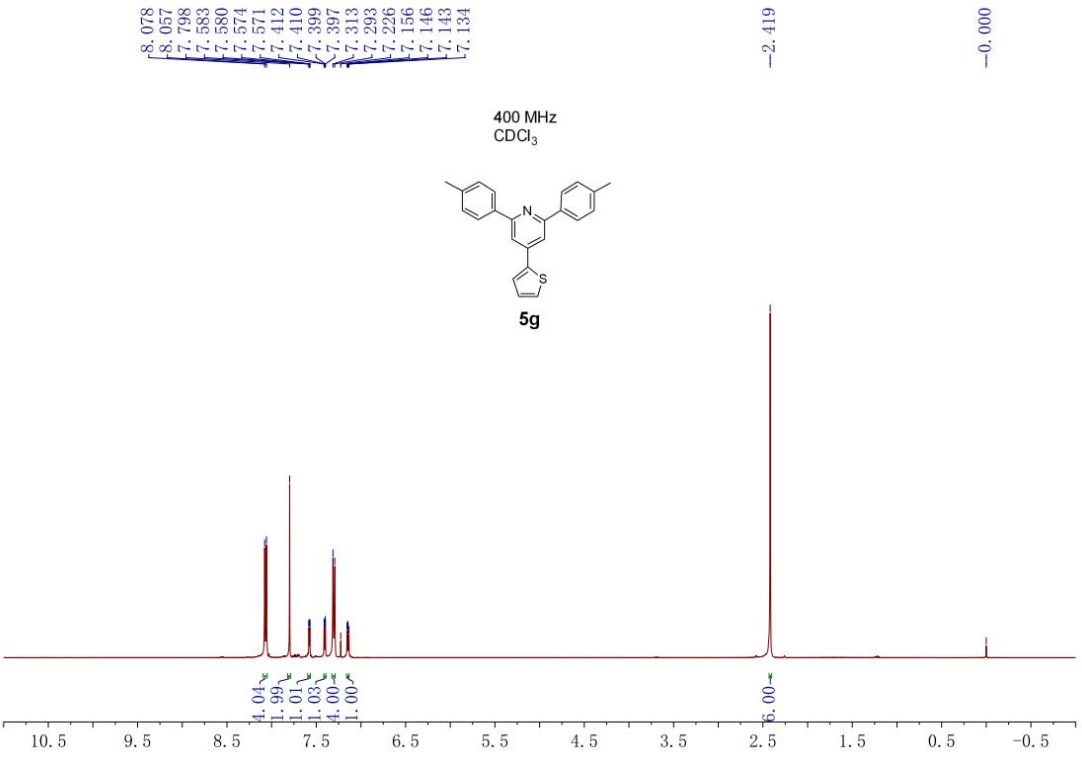

157.40
153.70
150.28
139.05
138.78
136.77
135.19
129.41
127.00
116.57
104.45
77.32
77.00
76.68
61.00
56.35
21.32
100 MHz
CDCl3
MeO
OMe
OMe
5d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

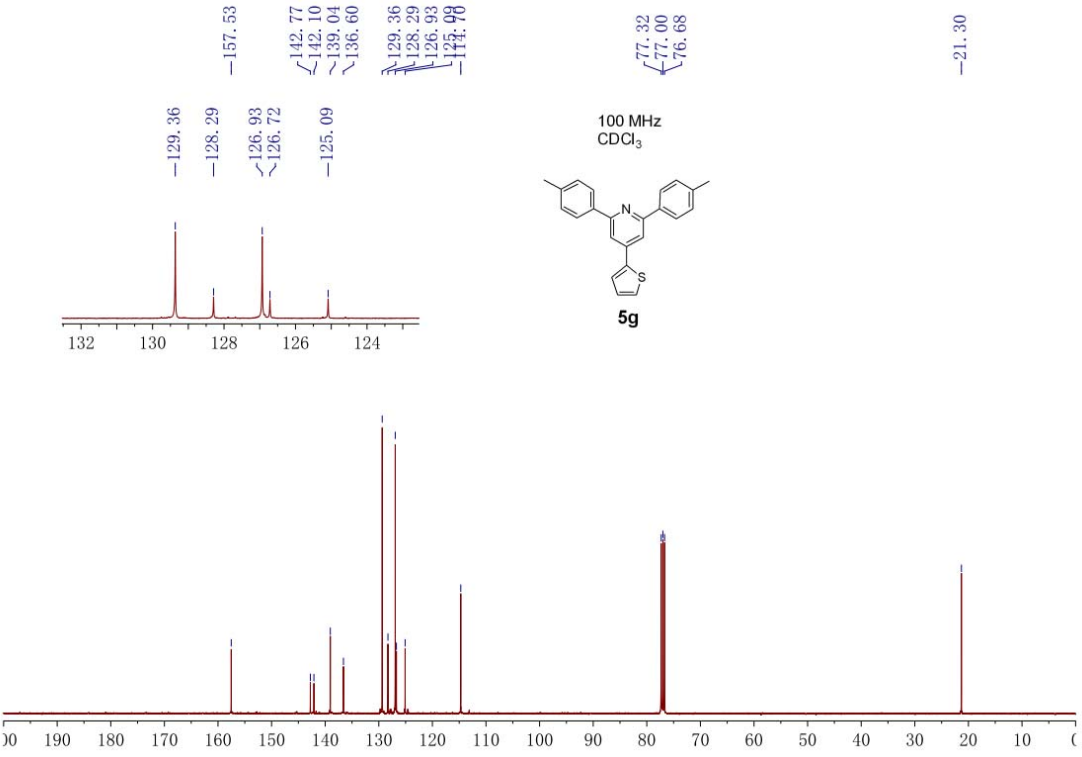

8.093
8.073
7.807
7.779
7.329
7.309
7.253
2.434
0.000
400 MHz
CDCl3
N
CN
5e
4.02
3.97
2.04
4.01
6.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5


157.75
148.00
143.72
139.37
136.31
132.82
129.48
127.90
126.94
118.53
116.19
112.51
77.32
77.00
76.68
21.32
100 MHz
CDCl3
N
CN
5e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


8.785
8.776
8.110
8.089
7.835
7.660
7.646
7.341
7.321
7.259
2.442
0.000
400 MHz
CDCl3
5f
2.04
4.02
2.01
2.01
3.99
6.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5


157.88
150.42
147.15
146.88
139.39
136.35
129.50
126.97
121.74
116.00
77.32
77.00
76.68
21.33
100 MHz
CDCl3
5f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


8.078
8.057
7.798
7.583
7.580
7.574
7.571
7.412
7.410
7.399
7.397
7.313
7.293
7.226
7.156
7.146
7.143
7.134
2.419
0.000
400 MHz
CDCl3
5g
4.04
1.99
1.01
1.03
4.00
1.00
6.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5


157.53
142.77
142.10
139.04
136.60
129.36
128.29
126.93
125.09
77.32
77.00
76.68
21.30
129.36
128.29
126.93
126.72
125.09
100 MHz
CDCl3
5g
132
130
128
126
124
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10